Program & Abstracts

50th Vietnam Conference on Theoretical Physics

HỘI NGHỊ VẬT LÝ LÝ THUYẾT VIỆT NAM LẦN THỨ 50

Dalat

4 - 7 August 2025

Program & Abstracts

50th Vietnam Conference on Theoretical Physics

Dalat Palace Heritage Hotel
02 Tran Phu Street,
Dalat, Lâm Đồng, Vietnam

4-7 August, 2025

Contents

Welcome Message

It is a great pleasure to welcome you in the 50th Vietnam Conference on Theoretical Physics (VCTP-50).

The VCTP-50 is organized by the Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST) under the support of the Vietnam Theoretical Physics Society (VTPS). It is sponsored by International Centre of Physics (ICP) at the Institute of Physics, VAST in Hanoi, Vietnam and Asia Pacific Center for Theoretical Physics (APCTP) in Pohang, Korea.

The VCTP, formerly known as the National Conference on Theoretical Physics (NCTP), has been an annual activity of VTPS since 1976. The VCTP is aimed to be an international conference for physicists in Vietnam, in the region and worldwide. Our mission is to foster scientific exchanges and to promote a high-standard level of research and education in Vietnam and in the South East Asia region.

This year, the VCTP conference is participated by nearly 175 participants. 10 invited talks, 35 oral and 107 poster contributions will be presented. We acknowledge the supports of the ICP conference program and the APCTP external program [APCTP-2025-E08].

We wish you enjoy the scientific atmosphere at this conference.

The Organizing Committee

Committees

Organizer

- Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST)

Organizing Committee

- Tran Minh Tien (Institute of Physics, VAST), Chair
- Trinh Xuan Hoang (Institute of Physics, VAST)
- Do Thi Huong (Institute of Physics, VAST)
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- Chu Thuy Anh (Institute of Physics, VAST, Hanoi)

Sponsors

- International Centre of Physics (ICP), Institute of Physics, Vietnam Academy of Science and Technology
- Asia Pacific Center for Theoretical Physics (APCTP)

General Information

Conference venue

The VCTP-50 conference takes place in:

Dalat Palace Heritage Hotel
02 Tran Phu Street,
Dalat, Lâm Đồng, Vietnam

Instructions for participation

- Participation takes place at the conference site.
- Oral presenters present their talks as in a normal conference.
- Poster presenters present the posters as in a normal conference.

Instructions for speakers

The duration of a regular invited talk is 40 minutes. This includes 35 minutes for the presentation itself and 5 minutes for Q&A. The duration of a regular presentation is 25 minutes. This includes 22 minutes for presentation itself and 3 minutes for Q&A. We would appreciate it if all presenters can adhere strictly to these time limits.

Instructions for Posters

Poster should be prepared as one page of size A0 (841 mm x 1189 mm) in portrait (vertical) mode. The presenting author of the poster should be present during the poster session.

Meeting room

All sessions take place in the Le Princess & Le Royal conference room of the Dalat Palace Heritage Hotel. Please follow the direction in the lobby to go to the conference room.

Lunches

Lunches are provided for conference participants in the Dalat Palace Heritage Hotel. Lunch coupons are included in your name badge holder. Extra coupons (limited in number) may be purchased for accompanied family members at the registration desk.

Gala dinner

All offline participants are invited to the Gala dinner:

Time: 6 August 2025, from 18:30

For your family members to attend the Gala Dinner, please buy tickets from the conference secretary on 4 August.

VTPS Meeting

A regular meeting of the Vietnamese Theoretical Physics Society (VTPS) will be held on the first day of the conference.

Time: 17:30 - 18:00, Monday, 4 August 2025.
Place: Le Princess & Le Royal conference room, Dalat Palace Heritage Hotel.

VTPS Young Researcher Award

At the opening session of the conference, there will be an announcement and the delivery of the 2025 VTPS Young Researcher Award.

Program timetable

Time	Monday, 4 August	Tuesdat, 5 August		Wednesday, 6 August	Thursday, 7 August	
08:30 – 10:00	Registration (8:30) Opening (9:00) VTPS Young Researcher Award Trieu D. An (I.1) Photo Session *(Chair: Tran Minh Tien)*	Poster Session 1 *(Chair:Trinh Xuan Hoang)*			Poster Session 2 *(Chair: Nguyen Hong Quang)*	
10:00 – 10:30	Coffee break	Coffee break			Coffee break	
10:30 – 12:00	Y. Morikawa (I.2) Nguyen Ngoc Linh (O.1) Nguyen Duc Long (O.2) *(Chair: Jer-Lai Kuo)*	N. Volchanskiy (I.5) Senaha Eibun (O.6) Lott Peter Tell (O.7) *(Chair: Cao Van Son)*	Ching-Ming Wei (I.6) Do Ngoc Son (O.8) Vo Khuong Dien (O.9) *(Chair: Nguyen N. Linh)*		Chavis Srichan (O.20) Nguyen L. T. Ngan (O.21) Nguyen H. K. Ngan (O.22) *(Chair: Ngoc -Loan Phan)*	Yang Zhesen (I.9) R.C.F Caballar (O.23) Dinh Thi Nguyen (O.24) *(Chair: T. T. K. Nguyen)*
12:00 – 14:00	Lunch	Lunch		Excursion	Lunch	
14:00 – 15:30	Hoang Ngoc Long (I.3) Do Thi Huong (O.3) Tran Van Que (O.4) *(Chair: Phung Van Dong)*	Ngoc-Loan Phan (I.7) H. Mineo (O.10) Tran Dong Xuan (0.11) *(Chair: Tran Nguyen Lan)*	Ki-Seok Kim (I.8) Thanh T. K. Nguyen (O.12) H. T. M. Nghiem (O.13) *(Chair:Tran Minh Tien)*		Nguyen Q. Hung (I.10) Le Tan Phuc (O.25) Cao Van Son (O.26) *(Chair: Le Duc Ninh)*	Le Nhat Thanh (O.27) N. T. T. Nhung (O.28) Nguyen Van Thu (O.29) *(Chair: Phan Van Nham)*
15:30 – 16:00	Coffee break	Coffee break			Coffee break	
16:00 – 17:30	Jer-Lai Kuo (I.4) Tran Nguyen Lan (O.5) 50th Aniversary of VTPS *(Chair: Le Van Hoang)*	Phung Van Dong (O.14) Tran Minh Hieu (O.15) Do Quoc Tuan (O.16) *(Chair:Do Thị Huong)*	Le Thu Lam (O.17) Nguyen Ba Phi (O.18) Phong H. Nguyen (O.19) *(Chair:Nguyen T. Tien)*		Nguyen T.B. Trang (O.30) Tran C. Minh (O.31) Luong Le Hai (O.32) *(Chair: Hoang Anh Tuan)*	N.-T. T. Hieu (O.33) Tung D. Nguyen(O.34) Pham N. Thanh (O.35) *(Chair: Do Ngoc Son)*
	VTPS Meeting **(17:30)**			Gala dinner **(19:00)**	Closing	

Acknowledgement notice

The 50th Vietnam Conference on Theoretical Physics is sponsored in part by the Asia Pacific Center for Theoretical Physics (APCTP). The APCTP kindly requests that participants acknowledge it in their work where APCTP has played a role. The number assigned to the 50th Vietnam Conference on Theoretical Physics is: [APCTP-2025-E08]. Below are some suggested templates for acknowledgment that participants may use:

- This work was initiated at the external program [APCTP-2025-E08] held at Dalat City, Vietnam.
- We thank the participants of the external program [APCTP-2025-E08] held at Dalat City, Vietnam for fruitful discussions.
- We thank APCTP, Pohang, Korea, for their hospitality during the External Program [APCTP-2025-E08], from which this work greatly benefited.

Conference Program

Monday, 4 August 2025

Opening Session
Chair: Tran Minh Tien

08:30 - 09:00	Registration
09:00 - 09:10	Opening
09:10 - 09:20	Announcement of 2025 VTPS Young Researcher Award
09:20 - 10:00	I.1 – Invited Manifestation of laser-target symmetry breaking in high-harmonic generation: from frequency shift to odd-even intensity modulation. **Trieu Doan An** (Institute of Fundamental and Applied Sciences, Duy Tan University)
10:00 - 10:10	Photo Session
10:10 - 10:30	Coffee break

Oral Session 1: *Condensed Matter Physics*
Chair: Jer-Lai Kuo

10:30 - 11:10	I.2 – Invited Origin for the Colossal Permittivity in Nb-doped TiO2 **Morikawa Yoshitada** (The University of Osaka)
11:10 - 11:35	O.1 – Oral When a defect in materials is a good thing? **Nguyen Ngoc Linh** (Faculty of Materials Science and Engineering, Phenikaa University)
11:35 - 12:00	O.2 – Oral Structure Prediction in the Search for Hydride-Based High-Temperature Superconductors **Nguyen Duc-Long** (Science and Technology Advanced Institute, Van Lang University)
12:15 - 14:00	Lunch

Oral Session 2: *Particle, Nuclear and Astrophysics*
Chair: Phung Van Dong

14:00 - 14:40 I.3 – Invited
Rare decay of axion to pair of photons in 3-3-1 model with Peccei-Quinn symmetry
Hoang Ngoc Long (STAI, VLU)

14:40 - 15:05 O.3 – Oral
$U(1)_N$ as a common source for light fermionic dark matter and radiative neutrino masses
Do Thi Huong (Institute of Physics)

15:05 - 15:30 O.4 – Oral
Refining Gravitational Wave and Collider Physics Dialogue via Singlet Scalar Extension
Tran Van Que (NCTS, National Taiwan University)

15:30 - 16:00 Coffee break

Oral Session 3: *Condensed Matter Physics*
Chair: Le Van Hoang

16:00 - 16:40 I.4 – Invited
Understanding Quantum Resonance through IR spectroscopy and Ab Initio Anharmonic algorithms
Kuo Jer-Lai (IAMS, Academia Sinica)

16:40 - 17:05 O.5 – Oral
Quantum many-electron simulation: from correlated mean-field to quantum computing
Tran Nguyen Lan (University of Science, VNU-HCM)

17:05 - 18:00 VTPS meeting

Tuesday, 5 August 2025

Poster Session 1
Chair: Trinh Xuan Hoang

08:30 - 10:00 P.1 – Poster
Impact of Channel Asymmetry on Thermoelectric Transport in a Two-Channel Charge Kondo System
Nguyen Hong Quang (Institute of Physics, Vietnam Academy of Science and Technology)

08:30 - 10:00 P.2 – Poster
Stochastic generation of magnetization in the one-dimensional Ising model exposed to Gaussian white, Brownian red, and pink noises
Villegas Paat Vladimir (Department of Physics, School of Foundational

Studies and Education, Mapua University)

08:30 - 10:00 P.3 – Poster

Molecular Simulation-Assisted Aptamer Selection for Lipopolysaccharide Detection and Development of a Simple Electrochemical Aptasensor

Nguyen Hai Ly (Duy Tan University)

08:30 - 10:00 P.4 – Poster

Density Functional Theory Analysis of CH_4 and Its Halogenated Derivatives Adsorption Behavior on SnPb Surface for the Development of Gas Sensors

Tung Thanh Nguyen (Institute of Engineering Technology, Thu Dau Mot University)

08:30 - 10:00 P.5 – Poster

Metal-insulator transitions in the two-dimensional ionic Hubbard model within coherent potential approximation.

Nguyen Yen (Institute of Physics, VAST)

08:30 - 10:00 P.6 – Poster

Electromagnetically Induced Transparency in GaAs/InAs Quantum Wells under Magnetic Field and Phonon Interaction

Tran Cong Phong (Ton Duc Thang University)

08:30 - 10:00 P.7 – Poster

Tracking Diamond Tool Wear in Iron Machining with Machine Learning Simulation Study

Nguyen Trinh Bao Anh (The University of Osaka)

08:30 - 10:00 P.8 – Poster

Theoretical elucidation of local atomic structures and colossal permittivity properties of Nb-doped TiO_2

Dinh Ngoc Dung (The University of Osaka)

08:30 - 10:00 P.9 – Poster

Monte Carlo Simulation of Magnetocaloric Effects in Doped Perovskites

Nguyen Thi Phuong Thuy (Institute of Physics, VAST)

08:30 - 10:00 P.10 – Poster

In silico ion-gated targeting treatment of selected diseases using a stochastically-reset Ising model

Lamento-Villegas Barbarona Em-Em (Philippine Eye Research Institute, National Institutes of Health, University of the Philippines Manila)

08:30 - 10:00 P.11 – Poster

Boundary Effects and Symmetry Breaking in Maxwell–Chern–Simons Theory

Nguyen Huu Ha (University of Dalat)

08:30 - 10:00 P.12 – Poster

The universe as a Grand computational System

Matthew Stanley Leibel (NA)

08:30 - 10:00 P.13 – Poster

The nernst coefficient in semi-parabolic plus semi-inverse squared quantum wells under the influence of intense electromagnetic waves

Nguyen Quang Son (Air Defence-Air Force Academy)

08:30 - 10:00 P.14 – Poster

The transfer of quantum entanglement in a rhombic spins system

Le Duc Vinh (Tinh Gia 3 High School)

08:30 - 10:00 P.15 – Poster

Many-Body Effects and Velocity Renormalization in Doped Monolayer MoS_2

Le Van Tan (Van Lang University)

08:30 - 10:00 P.16 – Poster

Tuning electronic and magnetic properties of semiconducting silicon carbide nanoribbons using hydrogen doping: A first-principles investigation

Dang Phuc Dam (College of natural sciences, Can Tho University)

08:30 - 10:00 P.17 – Poster

Diverse electronic and magnetic properties of silicon-doped graphene nanoribbons: A hybrid functional study

Nguyen Duy Khanh (Institute for Computational Science and Artificial Intelligene, Van Lang University)

08:30 - 10:00 P.18 – Poster

Electrochemical performance study of a full-cell Lithium-ion battery using a Bi2O3@NaBi(MoO4)2 anode and LiCoO2 cathode

Nguyen Tuan Loi (Duy Tan University)

08:30 - 10:00 P.19 – Poster

Study of the thermodynamic properties of SrZrO3 perovskite by the statistical moment method

Cao Huy Phuong (Hung Vuong High School for the Gifted)

08:30 - 10:00 P.20 – Poster

Nghiên cứu dự đoán cấu trúc Janus hai chiều SnSO và ảnh hưởng của pha tạp kim loại chuyển tiếp lên các tính chất điện tử và từ tính của nó

Do Minh Hoat (Duy Tan University)

08:30 - 10:00 P.21 – Poster

The breaking of $\mu - \tau$ reflection symmetry in a $B - L$ model with $(Z_2 \times Z_4) \rtimes Z_2\,(II)$ symmetry

Vo Van Vien (Tay Nguyen University)

08:30 - 10:00 P.22 – Poster

Electronic phase diagram of the half-filled ionic Hubbard model on the honeycomb lattice

Hoang Anh-Tuan (Institute of Physics, VAST)

08:30 - 10:00 P.23 – Poster

Optical Force Modulation on Monolayer Graphene in Microcavities: Graphene as a Medium vs. an Interface

Le Tri Dat (Dong Nai Technology University)

08:30 - 10:00 P.24 – Poster

Two dimensional Semi-Parabolic Plus Semi-Inverse Squared Quantum Well: Theoretical study of the oscillation in the quantum Ettingshausen effect at low temperature under the influence of intense electromagnetic waves.

Nguyen Dinh Nam (Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam)

08:30 - 10:00 P.25 – Poster

Size and shape effects on electronic properties of CdX (X=Te, Se, and S) semiconductor nanoparticles

Ho Khac Hieu (Duy Tan University)

08:30 - 10:00 P.26 – Poster

Half-metal state in honeycomb lattice with defects

Nguyen Hong-Son (Trade Union University)

08:30 - 10:00 P.27 – Poster

This computational research delves into the electronic, magnetic, and spin transport phenomena observed in rich spin penta-PdSe2 nanoribbons

Nguyen Hai Dang (Nam Can Tho University)

08:30 - 10:00 P.28 – Poster

The Debye-Callaway model for thermal conductivity calculation of black phosphorus nanoribbons

Nguyen Viet Chien (Phenikaa University)

08:30 - 10:00 P.29 – Poster

Design and Optimization of Multilayer Metamaterial Perfect Absorbers for Broadband Solar Energy Harvesting

Do Thi Nga (Institute of Physics, VAST)

08:30 - 10:00 P.30 – Poster

Collective excited states at small amplitude in neutron elastic scattering at low-energies

Do Quang Tam (University of Medicine and Pharmacy, Hue University)

08:30 - 10:00 P.31 – Poster

First-Principles Study of Hydrogen Cyanide Captured on M2CO2 (M = Sc, Ti, V) MXenes

Le Nguyen-Minh Thong (Institute for Advanced Study in Technology, Ton Duc Thang University)

08:30 - 10:00 P.32 – Poster

Qutrit-based simulation of collective three-flavor neutrino oscillations

Vũ Văn Hướng (Hanoi National University Education)

08:30 - 10:00 P.33 – Poster

The Dimerization of the Aβ42 under the Influence of the Gold Nanoparticle: A REMD Study

Ngo Son Tung (Institute for Advanced Study in Technology, Ton Duc Thang University)

08:30 - 10:00 P.34 – Poster

Optical transitions and Hofstadter spectra of monolayer TMDCs: a tight-binding investigation

Tran Khoi Nguyen (Department of Physics, University of Science, Vietnam National University Ho Chi Minh City)

08:30 - 10:00 P.35 – Poster

Regulated perturbation theory for anisotropic 2d exciton and a variable separation procedure for complicated double integrals

Le Do Dang Khoa (HCMUE)

08:30 - 10:00 P.36 – Poster

Dynamical Optical Absorption of a Monolayer Graphene inside an Empty Optical Microcavities

Pham Nguyen Thanh Vinh (Ho Chi Minh City University of Education)

08:30 - 10:00 P.37 – Poster

Two-component dark matter from a flavor-dependent U(1) extension of the standard model

Duong Van Loi (Phenikaa University)

08:30 - 10:00 P.38 – Poster

Effect of temperature and pressure on thermodynamic and melting properties of HP2 structure thallium metal

Nguyen Thi Hong (Hong Duc university)

08:30 - 10:00 P.39 – Poster

Neutrinoless double beta decay in an extended model with left-right symmetry

Dinh Nguyen Dinh (Institute of Physics)

08:30 - 10:00 P.40 – Poster

Controlling displacement of warp drive spaceship system using Proportional-Integral-Derivative controller

Trần Đình An (Ho Chi Minh City University of Technology and Education)

08:30 - 10:00 P.41 – Poster

Electronic and thermoelectric properties of WO3 under the adsorption of volatile organic compounds: first-principle study

Phan Thi Hong Hoa (Ho Chi Minh City University of Technology)

08:30 - 10:00 P.42 – Poster

Light absorbed by Dirac electrons in silicene under a non-uniform magnetic field

Huynh V. Phuc (Dong Thap University)

08:30 - 10:00 P.43 – Poster

The Hall Effect in an infinite Semi-parabolic Plus Semi-inverse Squared Quantum wells in the presence of a Strong Electromagnetic Wave.

Bui Thi Dung (Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam)

08:30 - 10:00 P.44 – Poster

`Darksuite`: an Algorithm for Dark-Matter Admixed Neutron Stars

Nguyen Thi Lan Anh (Phenikaa University)

08:30 - 10:00 P.45 – Poster

Modeling Myopia Progression through an Evolution Equation: Interactions Between Stimulus, Attention, and Eye Elasticity

Nguyễn Văn Hoa (GV)

08:30 - 10:00 P.46 – Poster

Interface Engineering and Electric Contact Design of two-dimensional van der Waals Heterostructure for Flexible Electronics

Nguyễn Văn Chương (Le Quy Don Technical University)

08:30 - 10:00 P.47 – Poster

Elucidating H_2S adsorption on activated carbon by van der Waals corrected density functional theory calculations

Nguyen Le Bao Tran (Quy Nhon University)

08:30 - 10:00 P.48 – Poster

Retrieving Anharmonic Interatomic Potentials from Conventional and Laser-Induced Electron Diffraction

Nguyễn Thị Hiền (Tay Nguyen University)

08:30 - 10:00 P.49 – Poster

Impact of nuclear reaction cross sections on primordial deuterium abundance

Dao Nhut Anh (Ho Chi Minh City University of Education)

08:30 - 10:00 P.50 – Poster

Emergent Localized Electronic States and Phonon Suppression in V_2WO_6: A New Class of Oxide Thermoelectric Materials

Le Nguyen Ngoc Quy (University of Science - VNUHCM)

08:30 - 10:00 P.51 – Poster

$(g-2)_{e,\mu}$ and lepton flavor violating decays in a left-right model

Nguyen Hua Thanh Nha (Van Lang University)

08:30 - 10:00 P.52 – Poster

Orientation asymmetry of planar molecules reflected in high-harmonic generation spectra

Trần Thành (Ho Chi Minh City University of Education)

08:30 - 10:00 P.53 – Poster

Studying nonclassical properties of the superposition of photon-added and

photon-subtracted single-mode displaced Fock state
Ho Sy Chuong (Dong Nai University)

08:30 - 10:00 P.54 – Poster
Investigation of thermodynamic properties of ideal classical and quantum gases in one-, two-, and three-dimensional space.
Phan Quang Sơn (University of Science, VNU-HCM)

10:00 - 10:30 Coffee break

Oral Session 4A: *Particle, Nuclear and Astrophysics*
Chair: Cao Van Son

10:30 - 11:10 I.5 – Invited
Renormalon-chain contributions to evolution kernels and two-point correlators of nonlocal quark currents
Volchanskiy Nikolay (Bogoliubov Laboratory of Theoretical Physics, JINR, Russia)

11:10 - 11:35 O.6 – Oral
Exploring CP Violation and EDM Cancellation in a Scale-Invariant g2HDM
Senaha Eibun (Van Lang University)

11:35 - 12:00 O.7 – Oral
Gravitational-Wave Signatures of the Kozai-Lidov Effect
Lott Peter Tell (Phenikaa University)

Oral Session 4B: *Condensed Matter Physics*
Chair: Nguyen Ngoc Linh

10:30 - 11:10 I.6 – Invited
Exploring structures and dynamics of materials with mobile atoms using machine-learning interatomic potential
Ching-Ming Wei (Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan)

11:10 - 11:35 O.8 – Oral
Capture, conversion, and utilization of hydrocarbon fuel from carbon dioxide: A case study
Do Ngoc Son (Ho Chi Minh City University of Technology)

11:35 - 12:00 O.9 – Oral
Tunable Thermal Transport in Hole-Doped Monolayer Penta-Graphene: A First-Principles and Machine Learning Study
Vo Khuong Dien (FPT University, Can Tho Campus)

12:00 - 14:00 Lunch

Oral Session 5A: *Molecular Physics, Quantum Optics and Quantum Information*
Chair: Tran Nguyen Lan

14:00 - 14:40 I.7 – Invited

Terahertz-Assisted High-Order Harmonic Generation for Waveform Sampling and Coherent XUV Emission
Phan Ngoc-Loan (Ho Chi Minh City University of Education)

14:40 - 15:05 O.10 – Oral
Theoretical study of a quantum control to create the photon-dressed states using pump lasers
Mineo Hirobumi (Van Lang University)

15:05 - 15:30 O.11 – Oral
Quantum Batteries VS Lithium-ion battery
Tran Dong Xuan (Duy Tan University)

Oral Session 5B: *Condensed Matter Physics*
Chair: Tran Minh Tien

14:00 - 14:40 I.8 – Invited
Dual holography from a non-perturbative generalization of the Wilsonian RG framework
Ki Seok Kim (POSTECH)

14:40 - 15:05 O.12 – Oral
Thermoelectric transport in some charge Kondo circuits: Generalized Cutler-Mott relation
Nguyen Thi Kim Thanh (Institute of Physics, VAST)

15:05 - 15:30 O.13 – Oral
TDNRG approach to work distributions for quantum impurity systems
Nghiem Hoa (Phenikaa University)

15:30 - 16:00 Coffee break

Oral Session 6A: *Particle, Nuclear and Astrophysics*
Chair: Do Thi Huong

16:00 - 16:25 O.14 – Oral
Towards a dark grand unification
Phung Van Dong (Phenikaa University)

16:25 - 16:50 O.15 – Oral
Type-I two Higgs doublet model: current data fitting and future detection ability
Tran Minh Hieu (Hanoi University of Science and Technology)

16:50 - 17:15 O.16 – Oral
Dimensional reduction issue of a six-dimensional Kaluza-Klein theory
Do Quoc Tuan (Phenikaa University)

Oral Session 6B: *Condensed Matter Physics*
Chair: Nguyen Thanh Tien

16:00 - 16:25 O.17 – Oral

Understanding the mechanism of the co-doping effect on ionic conductivity of Gd3+ and M3+ (M = Nd, Pr) co-doped ceria for solid oxide fuel cell applications
Le Thu Lam (Tay Bac University)

16:25 - 16:50 O.18 – Oral
Phase transitions in Hatano–Nelson lattice chains with periodically modulated disorder
Nguyen Ba Phi (Mientrung University of Civil Engineering)

16:50 - 17:15 O.19 – Oral
First-order magnetic transition and giant magnetic entropy change induced by random anisotropy in external fields
Nguyen Hai Phong (University of Science, Vietnam National University)

Wednesday, 6 August 2025

08:00 - 16:00 Excursion

19:00 - 21:00 Gala dinner

Thursday, 7 August 2025

Poster Session 2
Chair: Nguyen Hong Quang

08:30 - 10:00 P.55 – Poster
A renormalizable neutrino mass model with $(Z_2 \times Z_4) \rtimes Z_2$ (II) symmetry
Trần Đình Thám (Trường Đại học Phạm Văn Đồng)

08:30 - 10:00 P.56 – Poster
The effect of oxygen vacancy concentration on structural, electronic and optical properties of Bi_2WO_6 photocatalyst: DFT study
Doan Thi Hien (Hanoi National University of Education)

08:30 - 10:00 P.57 – Poster
Modeling Gravitational Wave Signatures from Magnetars Using Generally-Relativistic Magnetohydrodynamic Simulations
Nguyen Thi Thao Trang (Phenikaa University)

08:30 - 10:00 P.58 – Poster
Solving bound and scattering problems using symmetric matrix techniques
Nguyen Gia Huy (Ho Chi Minh City University of Education (HCMUE), Ho Chi Minh City)

08:30 - 10:00 P.59 – Poster
Reflection coefficient of a superconducting artificial atom coupled to a mirror
Tran Thi Thanh Huyen (Hanoi National University of Education)

08:30 - 10:00 P.60 – Poster

Evaluation of nuclear level density dependence on quadrupole deformation in ^{56}Fe nuclei

Le Thi Quynh Huong (University of Khanh Hoa)

08:30 - 10:00 P.61 – Poster

Thermoelectric properties in tilted 8-Pmmn borophene

Bui Dinh Hoi (Hue University of Education)

08:30 - 10:00 P.62 – Poster

Optically controlled spin transport in topological insulator thin films

Le Thi Thu Phuong (Hue University of Education)

08:30 - 10:00 P.63 – Poster

Molecular mechanism of Ensitrelvir and its similarity inhibiting SARS-CoV-2 main protease by molecular dynamics simulation

Nguyen Quoc Thai (Dong Thap University)

08:30 - 10:00 P.64 – Poster

Thermal fluctuations and mass imbalance impacts on excitonic-polaritonic condensation in a microcavity

Do Thi Hong Hai (Hanoi University of Mining and Geology)

08:30 - 10:00 P.65 – Poster

Molecular Simulation of Noble Gas Fractionation in CO_2-Water Systems under Geological Conditions

Nguyen Tu Khai Nam (Duy Tan University)

08:30 - 10:00 P.66 – Poster

Interfacial Tension of Carbon Dioxide – Water: A Molecular Simulation Study

Nguyen Ngoc Mai Phuong (Duy Tan University, Tan Tao University)

08:30 - 10:00 P.67 – Poster

Influence of Parameters on Structure, Phase Transitions, and Crystallization Processes of NiMn Alloys

Mai Van Dung (Thu Dau Mot University)

08:30 - 10:00 P.68 – Poster

First-principles insights into electron–phonon scattering limited mobility in two-dimensional Janus materials

Nguyễn Ngọc Hiếu (Đại học Duy Tân)

08:30 - 10:00 P.69 – Poster

BCS–BEC crossover of the equilibrium excitonic-polaritonic condensates in the mass imbalance optical microcavities

Nguyen Thi Hau (Hanoi University of mining and geology)

08:30 - 10:00 P.70 – Poster

Impact of laser parameters on photoisomerization probability in hydrogen cyanide

Lê Viết Nam (trường Đại học Sư phạm Thành phố Hồ Chí Minh)

08:30 - 10:00 P.71 – Poster

Study and design organic semiconductor materials with outstanding properties using New quantum computing methods

Trần Trí Nhân (Trường Đại học Khoa học Tự nhiên – ĐHQG TP.HCM)

08:30 - 10:00 P.72 – Poster

Scoto-seesaw model implied by flavor-dependent Abelian gauge charge

Nguyen Tuan Duy (Institute of Physics)

08:30 - 10:00 P.73 – Poster

Entanglement dynamics of an atom interacting with a generalized photon-added pair coherent state under phase damping

Le Thi Hong Thanh (Quang Nam University)

08:30 - 10:00 P.74 – Poster

Tracking nuclear vibration using mass spectrometry

Nguyen Dang Trong Thanh (Ho Chi Minh University of Education)

08:30 - 10:00 P.75 – Poster

Analytical method: Universal formula for obtaining fundamental material parameters of monolayer transition metal dichalcogenides from experimental exciton energies

Lê Hoàng Việt (HCMUE)

08:30 - 10:00 P.76 – Poster

Unraveling the electronic mechanisms of transition metal and fluorine codoping for enhanced electrochemical performance in sodium lithium manganese oxide cathodes

Nguyen Chi Ben (Can Tho University)

08:30 - 10:00 P.77 – Poster

A geometrical model for protein folding with directional interactions

Trinh Xuan Hoang (Institute of Physics, VAST)

08:30 - 10:00 P.78 – Poster

Study of Neutrino Masses from an A_4-Based Seesaw Model

Tran Tien Manh (IOP)

08:30 - 10:00 P.79 – Poster

Effect of polarized light and magnetic field on the transport properties of germanene

Do Muoi (Faculty of Natural Sciences, Pham Van Dong University, Quang Ngai)

08:30 - 10:00 P.80 – Poster

Enhanced Gas Sensing Performance via Au and B Co-doped Silicene/MoS2 Bilayer Heterostructures: A First-Principles Insight

Duong Trong Nhan (Van Lang University)

08:30 - 10:00 P.81 – Poster

Control of Superconducting Qubits

Nguyen Van Duy (Phenikaa University)

08:30 - 10:00 P.82 – Poster

Reaching High Accuracy for Energetic Properties at Second-Order Perturbation Cost by Merging Self-Consistency and Spin-Opposite Scaling

Nguyen Thanh Hoang (Institute of Advanced Technology - Vietnam Academy of Science & technology)

08:30 - 10:00 P.83 – Poster

Electric field enhances the electronic and diffusion properties of penta-graphene nanoribbon anodes in lithium-ion batteries

Nguyen Vo Anh Duy (FPT High School Can Tho, FPT University)

08:30 - 10:00 P.84 – Poster

Probing charge migration of molecular ion from high-harmonic spectra

Nguyen Thanh Dinh Duy (Ho Chi Minh City University of Education)

08:30 - 10:00 P.85 – Poster

Study of a single oxygen adatom on graphene using density functional theory

Tạ Văn Nam (Faculty of Materials Science and Engineering, Phenikaa University)

08:30 - 10:00 P.86 – Poster

Enhance sampling of amyloid beta peptide: the combination of molecular dynamics simulations and machine learning

Tran Thi Minh Thu (University of Science, Ho Chi Minh City)

08:30 - 10:00 P.87 – Poster

Unveiling HCN Isomerization Through HHG Spectrum Simulation

Huỳnh Thị Hải (Department of Physics, HCM University of Technology and Education)

08:30 - 10:00 P.88 – Poster

Research on stable phases in theoretical models for kagome magnetic materials.

Tran Thị Thanh Mai (Institute of Physics, VAST)

08:30 - 10:00 P.89 – Poster

Preliminary study of the correlation effects of a twisted bilayer structure of transition metal dichalcogenides

Nguyen Trong Son (Phenikaa University)

08:30 - 10:00 P.90 – Poster

Polarized ZZ pair production at the LHC: Theoretical status

Le Duc Ninh (Phenikaa University)

08:30 - 10:00 P.91 – Poster

Anharmonic high-order XAFS cumulants of crystalline silver within quantum-

statistical perturbation theory
Lê Việt Hoàng (Hanoi University of Science, Vietnam National University)

08:30 - 10:00 P.92 – Poster
Phase diagram for the pseudogap Kondo effect in graphene
Dang The Hung (Phenikaa University)

08:30 - 10:00 P.93 – Poster
Effect of dynamic core-electron polarization on High-order harmonic generation from oriented co molecules
Dam My Hoa (Ho Chi Minh City University of Education)

08:30 - 10:00 P.94 – Poster
Multielectron Effects in the High-Order Harmonic Generation Spectrum of Magnesium
Lê Trần Nhật Hào (Ho Chi Minh City University of Education)

08:30 - 10:00 P.95 – Poster
Constrain the free parameters of Lepton Flavor Symmetry Models with Neutrino Oscillation data
Phan To Quyen (IFIRSE, ICISE)

08:30 - 10:00 P.96 – Poster
Population imbalance driven Mott transitions in three-component Falicov-Kimball model
Tran Minh Tien (Institute of Physics, VAST)

08:30 - 10:00 P.97 – Poster
Statistical Analysis of Score Distribution Transitions in Non-Centralized Assessments: A Case Study of Final Exam
Chu Thuy Anh (Institute of Physics)

08:30 - 10:00 P.98 – Poster
Developing an Interactive Computational Platform for Molecule-Surface Material Interaction: Applying to Area Selective Atomic Layer Deposition simulations
Ngo Dang Huy (Phenikaa University)

08:30 - 10:00 P.99 – Poster
Dark matter relic abundance in an extended scalar sector with vector-like quarks
Nguyen Minh Hien (Faculty of Physics, University of Science, VNU-HCM)

08:30 - 10:00 P.100 – Poster
Investigation of the soft parameter in the electron-ion coulomb potential and the governing mechanisms of nonsequential triple ionization in noble gas atom
Chau Bao Khoa (Ho Chi Minh City University of Education)

08:30 - 10:00 P.101 – Poster
Searching for carbon cluster isomers using machine-learning potential

Nguyen Duy Huy (VNU University of Science, Vietnam National University, Hanoi)

08:30 - 10:00 P.102 – Poster

Tripeptides inhibit dual targets AChE and BACE-1: a computational study

Do Anh Tuan (Institute for Advanced Study in Technology, Ton Duc Thang University)

08:30 - 10:00 P.103 – Poster

An analytical approach to retrieving fundamental structural parameters of monolayer transition metal dichalcogenides from exciton spectra

Lý Duy Nhất (HCMC University of Education)

08:30 - 10:00 P.104 – Poster

Influence of local deformation on the adsorption of toxic gases on MoS2 monolayer: a first-principles investigation

Vương Khiết An (College of natural sciences, Can Tho University)

08:30 - 10:00 P.105 – Poster

Mechanical and electronic properties of TiVZrNbMox high entropy alloys: First principles calculations

Huynh Khanh Van (Can Tho University)

08:30 - 10:00 P.106 – Poster

Matching High Energy Scale Theory to Standard Model and Prediction of the Higgs Boson Mass

Dao Thi Nhung (Phenikaa University)

08:30 - 10:00 P.107 – Poster

Effects of laser parameters on orbital competition in high-order harmonic generation from hydrogen cyanide

Hoàng Trọng Đại Dương (Van Lang University)

10:00 - 10:30 Coffee break

Oral Session 7A: *Molecular Physics, Quantum Optics, and Quantum Information*
Chair: Phan Ngoc Loan

10:30 - 10:55 O.20 – Oral

Numerical Simulation of Black Hole to White Hole Transition Using Entangled Lattice-Based Qubits Formalism

Srichan Chavis (Faculty of Engineering, Khon Kaen University)

11:20 - 11:45 O.21 – Oral

Effects of boron or nitrogen dopants on electronic and optical properties of the graphene/h-BN heterostructure

Ngân Lưu Thanh Nguyễn (Ho Chi Minh City University of Technology - nltngan.sdh242@hcmut.edu.vn)

11:45 - 12:10 O.22 – Oral

Multielectron polarization-induced frequency shifts in high-order harmonic

generation: a manifestation of molecular asymmetry
Nguyen Huynh Kim Ngan (Duy Tan University)

Oral Session 7B: *Condensed Matter Physics*
Chair: Nguyen Thi Kim Thanh

10:30 - 11:10 I.9 – Invited
Theory for the non-Hermitian skin effect
Yang Zhesen (APCTP)

11:10 - 11:35 O.23 – Oral
Emergence of the Liouvillian Skin Effect in Driven – Dissipative Ultracold Atom Systems
Caballar F. Roland Cristopher (Department of Mathematics and Physics, College of Science, University of Santo Tomas)

11:35 - 12:00 O.24 – Oral
2D rotating Bose-Einstein condensation at the critical rotation speed
Nguyễn Đình Thi (University of Science, Vietnam National University Ho Chi Minh City, Vietnam)

12:00 - 14:00 Lunch

Oral Session 8A: *Particle, Nuclear and Astrophysics*
Chair: Le Duc Ninh

14:00 - 14:40 I.10 – Invited
Revisiting the anomaly in the production of 60Fe nucleus in massive stars
Nguyen Quang Hung (Institute of Fundamental and Applied Sciences, Duy Tan University)

14:40 - 15:05 O.25 – Oral
Possible existence of the pygmy dipole resonance built on excited states
Le Tan Phuc (IFAS, Duy Tan University)

15:05 - 15:30 O.26 – Oral
On the Leggett-Garg Inequality Testing with Neutrino Oscillation Measurements
Cao Van Son (IFIRSE, ICISE)

Oral Session 8B: *Soft Matter, Biological and Interdisciplinary Physics*
Chair: Phan Van Nham

14:00 - 14:25 O.27 – Oral
Thermoelectric properties of penta-InP_5: A first-principles and machine learning study
Lê Nhật Thanh (Trường Đại học Cần Thơ)

14:25 - 14:50 O.28 – Oral
Solvation effects on protein folding in a simple lattice model
Nguyen Thi Thuy Nhung (Graduate University of Science and Technol-

ogy)

15:50 - 15:15 O.29 – Oral
Degenerate points in wetting phase diagram of a dilute ternary Bose-Einstein mixtures
Nguyen Van Thu (Hanoi Pedagogical University 2)

15:30 - 16:00 Coffee break

Oral Session 9A: *Molecular Physics, Quantum Optics, and Quantum Information*
Chair: Hoang Anh Tuan

16:00 - 16:25 O.30 – Oral
Assessing the impact of ligand substitution on the optoelectronic properties and electron transport behavior of oligophenylene ethynylene
Nguyen Thi Bao Trang (Can Tho University)

16:25 - 16:50 O.31 – Oral
Investigating the Talbot effect in binary waveguide arrays
Trần Công Minh (Science and Technology Advanced Institute, Van Lang University)

16:50 - 17:15 O.32 – Oral
The Stark effect calculations in spherical coordinates
Luong Le Hai (Ho Chi Minh City University of Education)

Oral Session 9B: *Condensed Matter Physics*
Chair: Do Ngoc Son

16:00 - 16:25 O.33 – Oral
On Rydberg excitons in two-dimensional semiconductors
Nguyen-Truong T. Hieu (Van Lang University)

16:25 - 16:50 O.34 – Oral
Spin filtering in ring conductors by electromagnetic dressing
Nguyen Danh Tung (Institute of Physics)

16:50 - 17:15 O.35 – Oral
Machine learning enhanced global optimization and its application in elucidating hydrogen insertion in $SrMO_y$ (M = Fe and Co)
Pham Ngoc Thanh (An Giang University)

17:15 - 17:30 Closing

Conference Abstracts

I.1 – Invited, VCTP-50

Manifestation of laser-target symmetry breaking in high-harmonic generation: from frequency shift to odd-even intensity modulation

Doan-An Trieu (1,2)

(1) Duy Tan University, Ho Chi Minh City, Vietnam;
(2) Ho Chi Minh City University of Education, Ho Chi Minh City, Vietnam;

Although frequency shift and odd-even intensity modulation in high-order harmonic generation (HHG) have both been observed for asymmetric laser-target systems, they are typically studied as two separate effects. In this presentation, two investigations on the odd-even harmonics generation [1] and frequency shift [2] induced by a static electric field are reported, coming up with a general theory for unifying the two phenomena through a common origin and clarifying the controlling factor [3]. The theory is represented by a simple analytical model, and its generality is supported by numerical simulations with various asymmetric factors. Recognizing how asymmetry affects HHG helps us better understand the properties of the target material and supports applications such as mapping molecular dynamics or detecting subtle external fields.

References:

[1] Doan-An Trieu et al., Phys. Rev. A 108, 023109 (2023)

[2] Doan-An Trieu et al., Phys. Rev. A 110, L021101 (2024)

[3] Doan-An Trieu et al., Phys. Rev. A 110, L041101 (2024)

Presenter: Trieu Doan An

I.2 – Invited, VCTP-50

Origin for the Colossal Permittivity in Nb-doped TiO2

*Van An Dinh (1), Yujiro Hashimoto (2), Koji Kimura (3,4,5), Taro Kuwano (2), Dung Ngoc Dinh (1,6), Ryoji Asahi (2), Koichi Hayashi (3,4), *Hiroki Taniguchi (2), and *Yoshitada Morikawa (1)*
V.A.D. and Y.H. contributed equally to this work.

(1) The University of Osaka;
(2) Nagoya University;
(3) Nagoya Institute of Technology;
(4) Japan Synchrotron Radiation Research Institute (JASRI), SPring-8;
(5) National Institute for Materials Science;
(6) Graduate University of Science and Technology, Vietnam Academy of Science and Technology

We investigated the origin of colossal permittivity observed in Nb-doped rutile TiO2 using experimental and theoretical methods. Initially, we observed a significant enhancement of permittivity in Nb-doped TiO2, reaching up to 106. However, most of this enhancement diminishes below 20 K, indicating that it primarily arises from carrier redistribution at grain boundaries, so-called the Maxwell-Wagner effect. Even below 20 K, the permittivity remains around 103, four times higher than pristine TiO2. Additionally, the permittivity shows strong anisotropy, measuring approximately 1000 along the [001] direction and about 300 along the [110] direction. To clarify the physical mechanism behind the permittivity enhancement due to Nb singly doping in TiO2, we performed density functional theory (DFT) calculations using high-quality hybrid energy functionals. Our findings reveal that Nb dopant ionizes to form Nb5+ ion at a Ti site, donating electron to the TiO2 lattice, thereby forming polaron Ti3+. Doped Nb5+ ion and the polaron Ti3+ attract each other, and at low temperatures they localize at the first nearest neighbor sites along the [001] direction. The binding energy between Nb5+ ion and polaron Ti3+ is approximately 50 meV, indicating the formation of free polarons at temperatures above 20 K, contributing to colossal permittivity via the Maxwell-Wagner effect. Below 20 K, however, polarons are trapped at the first nearest neighbor sites of Nb5+ ions. Our DFT calculations using hybrid functionals suggest that the charge of the polaron distributes between the Nb5+ ion and the neighboring Ti ions, forming a molecular polaron. Despite being trapped near Nb dopant, the activation energy for polaron flip-flop motion between nearest neighbor Ti sites through Nb is only 15 meV, indicating unfrozen motion even at liquid helium temperatures. Based on these observations, we conclude that the significant permittivity enhancement observed at liquid helium temperatures originates from the flip-flop motion of molecular polarons facilitated by Nb dopants under an applied electric field. Moreover, we found strong mutual attraction between Nb ions that may cause the formation of Nb-Nb dimers within the TiO2 lattice. Consequently, increasing Nb dopant concentration may hinder the flip-flop motion at low temperatures. This is the origin for the saturation of permittivity observed experimentally at Nb concentrations around 1% or higher. Finally, to examine the local atomic arrangements around doped Nb, we conducted X-ray fluorescent holography experiments at 100 K. At low Nb concentrations (approximately 0.1%), Nb atoms showed negligible displacement from bulk Ti sites, whereas at higher concentrations (1%), significant Nb displacement was observed, supporting our hypothesis of single-doped Nb with free polarons at lower concentrations and Nb-Nb dimer formation at higher concentrations.

Presenter: Morikawa Yoshitada

I.3 – Invited, VCTP-50

Rare decay of axion to pair of photons in 3-3-1 model with Peccei-Quinn symmetry

H. N. Long (1), V. H. Binh (2)

(1) STAI, Van Lang University;
(2) IOP, VAST

In the frameworks of 3-3-1 model with Peccei-Quinn symmetry, axion state and anomaly couplings are derived. The decay of axion to pair of photons is considered. We show that anomaly coupling of axion gives suppressed contribution by one followed from Higgs sector.

Presenter: Hoang Ngoc Long

I.4 – Invited, VCTP-50

Understanding Quantum Resonance through IR spectroscopy and Ab Initio Anharmonic algorithms

Jer-Lai Kuo

Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

Normal modes and harmonic picture form a base to understand vibrational Hamiltonian. But Vibrational motions of molecules are intrinsically "anharmonic" and complex vibrational features in mid-IR associated with CH/NH/OH are often attributed to anharmonic coupling known as Fermi Resonance (FR). Our group has been devoted to develop ab initio anharmonic algorithms (A3) so that we can construct simple vibrational exciton models without any fitting parameters to understand FR and analyze experimental spectra of solvated H3O+ and CH3NH3+ in mid-IR.

Presenter: Kuo Jer-Lai

I.5 – Invited, VCTP-50

Renormalon-chain contributions to evolution kernels and two-point correlators of nonlocal quark currents

Nikolay Volchanskiy

Bogoliubov Laboratory of Theoretical Physics, Joint institute for nuclear research

We calculate ERBL evolution kernels and two-point massless QCD correlator of nonlocal composite vector and tensor quark currents with the chains of fermion one-loop radiative corrections inserted into gluon lines. The correlator depends on the Bjorken fraction x related to the composite current and, under large-β_0 approximation, gives the main contributions in each order of perturbation theory. In the approximation mentioned, these contributions dominate the endpoint behavior of the leading-twist distribution amplitudes of light mesons in the framework of QCD sum rules. Building upon these results, we analyze the endpoint behavior of these distribution amplitudes for pion and longitudinally polarized ρ mesons and find inequalities for their moments.

Presenter: Volchanskiy Nikolay

I.6 – Invited, VCTP-50

Exploring structures and dynamics of materials with mobile atoms using machine-learning interatomic potential

Ching-Ming Wei

Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

Various materials, such as superionic materials, lithium-ion batteries, and metal-organic frameworks, possess mobile atoms with liquid-like behavior in the rigid frameworks of other atoms. Experimentally, to reveal the detailed structures of mobile atoms is typically probed by a try-and-error fitting approach of X-ray Powder Diffraction (XPD) using the concept of partial occupancy. Since the mobile atoms diffuse very fast inside and between different crystal unit cells, limited numbers of partial occupancy cannot describe the details of the structures. To rescue this deficiency, we extend the concept of partial occupancy used at X-ray Powder Diffraction into continuous mode to define and obtain the three-dimensional atomic density distribution function (3D-ADDF) [1] of mobile atoms, which is easily obtained by performing reliable large-scale

molecular dynamics simulations. Conversely, the diffusion behavior of mobile atoms is usually probed by ab initio molecular dynamics simulations, where enormous computing resources are required for a complete thorough study. Thus, only limited cases are investigated without providing the most critical quantity, such as the diffusion constants and barriers. To address this shortcoming, we perform large-scale molecular dynamics simulations (up to 10 ns simulation times) based on machine-learning interatomic potentials, fitted from ab initio molecular dynamics simulations [2], to have complete studies for various materials: (i) superionic materials including Ag2S, Ag8SiTe6, Cu2S, Zn3.6+xSb3, and Cu7+xPS6; (ii) lithium-ion battery including LixCoO2, and Li6+xPS5Cl; (iii) metal-organic framework: H2O, CO2, N2, CH4 diffusion on [Ca(C4O4)(H2O)] (termed UTSA-280). Our results indicate that the Arrhenius equation can describe the diffusion behaviors of the various mobile atoms in the rigid framework very well, where the activation barriers range from 0.1 to 0.3 eV. The small diffusion barriers provide the fundamental origin for the liquid behaviors of mobile atoms.

References:

[1] C.-R. Hsing, D.-L. Nguyen, and C.-M. Wei, Phys. Rev. Mater. 6, 083601 (2022).

[2] C.-R. Hsing, D.-L. Nguyen, and C.-M. Wei, Phys. Rev. Mater. 8, 043806 (2024).

Presenter: Ching-Ming Wei

I.7 – Invited, VCTP-50

Terahertz-Assisted High-Order Harmonic Generation for Waveform Sampling and Coherent XUV Emission

Ngoc-Loan Phan (1), Doan-An Trieu (2), Van-Hoang Le (1)

(1) Ho Chi Minh City University of Education, Ho Chi Minh City, Vietnam;
(2) Duy Tan University, Da Nang, Vietnam

Terahertz (THz) fields—particularly THz pulses with durations ranging from picoseconds to nanoseconds—play a vital role in fundamental science, material control, and practical applications such as high-speed wireless communication technologies [1, 2]. Beyond generating THz pulses, accurately characterizing them is a critical step toward their full utilization. Among existing techniques, THz time-domain spectroscopy (THz-TDS) is widely used as it provides both amplitude and phase information of the THz field. However, THz-TDS remains technically challenging due to its strong dependence on the properties of the detection material, which limits its accuracy and measurable bandwidth [1, 2]. This motivates the development of alternative, material-independent methods for THz waveform sampling.

In this report, we demonstrate that high-order harmonic generation (HHG)—a nonlinear optical process emitted when atoms or molecules interact with an intense ultrashort laser field—can serve as a powerful and general tool for THz field characterization. When the laser interaction is assisted by a THz field, the resulting HHG spectrum encodes detailed information about the THz waveform through symmetry-breaking signatures. By establishing analytical relationships between the THz electric field and the odd-even harmonic intensity ratio or frequency shift in the HHG spectrum, we propose two universal THz-TDS methods [3-5]. The first measures the even-to-odd harmonic intensity ratio in atoms or symmetric molecules irradiated by a multicycle mid-infrared laser pulse [3]. The second extracts the frequency shift of harmonic peaks in the cutoff region using few-cycle laser pulses [4]. More specifically, we show that the two proposed methods are general and robust, being independent of the atomic or molecular species and laser parameters. This universality paves the way for a compact, all-optical scheme for THz waveform

sampling using standard tabletop HHG setups.

Additionally, we explore the potential of THz-assisted HHG for generating high-coherence extreme ultraviolet (XUV) and soft X-ray photons. We show that moderate THz fields can significantly extend the HHG cutoff, making it possible to achieve coherent high-energy radiation [6]. Such sources hold great promise for applications such as diagnosing microscopic defects in microelectronic components.

References:

[1]. X. C. Zhang, A. Shkurinov, and Y. Zhang, Nat. Photon. 11, 16 (2017).

[2]. Y. Zhang, K. Li, and H. Zhao, Front. Optoelectron. 14, 4 (2021).

[3]. D.-A. Trieu, N.-L. Phan, Q.-H. Truong, H. T. Nguyen, C.-T. Le, D. Vu, and V.-H. Le, Phys. Rev. A 108, 023109 (2023).

[4]. D.-A. Trieu, T.-T. D. Nguyen, T.-D. D. Nguyen, T. Tran, V.-H. Le, and N.-L. Phan, Phys. Rev. A 110, L021101 (2024).

[5]. D.-A. Trieu, V.-H. Le, and N.-L. Phan, Phys. Rev. A 110, L041101 (2024).

[6]. D.-A. Trieu, D. D. Hoang-Trong, C.-T. Le, S. Ha, V.-H. Le, and N.-L. Phan, in preparation.

Presenter: Phan Ngoc-Loan

I.8 – Invited, VCTP-50

Dual holography from a non-perturbative generalization of the Wilsonian RG framework

Ki-Seok Kim

Pohang University of Science and Technology, Korea

In my opinion, physics is to aim understanding the macroscopic universal IR physics from the microscopic individual UV physics based on the first principle. The Wilsonian renormalization group (RG) framework would be the first organization principle. Unfortunately, this theoretical framework has its limitation in describing many long-standing physics problems, where the RG flow from UV to IR is nonperturbative in nature and beyond the paradigm of spontaneous symmetry breaking. In this talk, we discuss how to generalize the Wilsonian RG framework in a nonperturbative way. First, we introduce a brute-force way of RG transformations. Remarkably, the resulting Wilsonian effective action contains a particular class (most singular) of quantum corrections in the all-loop order, not exact but completely nonperturbative in nature. We confirm this nonperturbative physics explicitly from the Kondo problem, which shows the asymptotic freedom (decoupled local moment fixed point) at UV and confinement (local Fermi liquid fixed point) at IR. Although this brute-force way of RG transformations is explicit, the intermediate procedure looks dirty and hidden, involved with the heat-kernel calculation in a general background. We realize that there exists a topological structure in this brute-force construction. Second, we discuss an elegant reformulation of the previous nonperturbative RG theoretical framework, referred to as a cohomological-type topological field theory construction a la Witten. We demonstrate that this topological reformulation is essentially the same as the previous explicit derivation. Interestingly, we observe that this cohomological construction gives a deep connection to the path integral representation of the exact functional RG equation, where the RG flow of the probability distribution function is governed by the Fokker-Planck-type equation. Based on this novel reformulation, we discuss Weyl anomaly inflow and cancellation for the resulting renormalized effective action, regarded to be the consistency equation for the non-

perturbative RG flow description. We see that all these mathematical structures are consistent with the holographic duality conjecture.

Presenter: Ki Seok Kim

I.9 – Invited, VCTP-50

Theory for the non-Hermitian skin effect

Yang Zhesen

Asia Pacific Center for Theoretical Physics, Pohang, Korea

The non-Hermitian skin effect, which represents a phenomenon where almost all the open boundary condition (OBC) eigenstates can be exponentially localized at the boundary, has drawn a lot of attention recently. From a theoretical viewpoint, building a theory to describe these exponentially-localized skin modes is a basic starting point at the first stage. For one-dimensional (1D) systems, this can be achieved by the generalized Brillouin zone (GBZ) theory, that is, both the OBC eigenvalues and eigenstates can be calculated analytically in the $N \to \infty$ limit. For 2D systems, although some efforts have been made to establish the corresponding GBZ theory, a universal framework is still lacking. In this talk, I will introduce our recent progress on the 2D GBZ theory, which can be applied to general 2D non-Hermitian systems under general OBC geometries.

Presenter: Yang Zhesen

I.10 – Invited, VCTP-50

Revisiting the anomaly in the production of ^{60}Fe nucleus in massive stars

Samapti Lakshan (1), Le Tan Phuc (2,3), Deepak Pandit (4, 5), Srijit Bhattacharya (6), Balaram Dey (1), Nguyen Ngoc Anh (7) and Nguyen Quang Hung (2,3)

(1) Department of Physics, Bankura University, Bankura, West Bengal, India;
(2) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City Vietnam;
(3) Faculty of Natural Sciences, Duy Tan University, Da Nang City, Vietnam;
(4) Variable Energy Cyclotron Centre, 1/AF-Bidhannagar, Kolkata, India;
(5) Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai, India;
(6) Department of Physics, Barasat Govt. College, Barasat, N 24 Pgs, Kolkata, India;
(7) Phenikaa Institute for Advance Study (PIAS), PHENIKAA University, Hanoi, Vietnam

A number of experiments have detected the presence of two long-lived ^{26}Al and ^{60}Fe radioisotopes and their ratio in both interstellar environments and terrestrial archives [1,2]. Those experimental detections provide fundamental probes for the nucleosynthesis in stars. In particular, a recent experiment, based on the gamma-decay spectroscopy of ^{60}Fe produced via the beta-decay of ^{60}Mn, has reported the enhanced production of ^{60}Fe in massive stars, which is almost 2 times higher than previous studies [3]. Such an enhanced production strongly impacts the ^{60}Fe/^{26}Al ratio, a primary source of uncertainties between gamma-ray telescope observations and supernova models. In this work, we revisit the ^{60}Fe production problem by analyzing the influence of nuclear physics uncertainties, typically the nuclear level density (NLD) and γ-rays strength function (gSF), on both the neutron-captured and Maxwellian averaged cross sections of (n,γ)^{60}Fe reaction. We show that both the partial (angular-momentum dependent) NLDs and low-energy gSF, which have not been measured, are the main sources that affect the ^{60}Fe

production.

References:

[1] W. A. Mahoney et al., Astrophys. J. 262, 742 (1982).

[2] W. R. Binns et al., Science 352, 677 (2016).

[3] A. Spyrou et al., Nat. Comm. 15, 9608 (2024).

Presenter: Nguyen Quang Hung

O.1 – Oral, VCTP-50

When a defect in materials is a good thing?

Ngoc Linh Nguyen (1), The Hung Dang (1), Tien Lam Pham (2) and Minh Hoa Nghiem (3)

(1) Faculty of Materials Science and Engineering, Phenikaa University;
(2) Faculty of Computer Science, Phenikaa University;
(3) Phenikaa Institute for Advanced Study, Phenikaa University

Defects in materials play a crucial role in determining their physical and chemical properties. Understanding and engineering these defect structures provide an effective strategy for tailoring materials for a wide range of applications, including photocatalysis, light emission, and quantum computing. In this talk, I will present our recent studies [1,2] on defects in cubic boron nitride (c-BN) aimed at developing novel solid-state quantum bits (qubits). Using first-principles simulations, we designed potential qubit-related defects in c-BN and computed key parameters such as the zero-phonon line, zero-field splitting, and hyperfine interactions. Our results are benchmarked against both experimental data and previous theoretical studies. The insights gained from this work offer valuable guidance for the design and optimization of defect-based qubits in c-BN, contributing to the advancement of solid-state quantum technologies.

References:

[1] Ngoc Linh Nguyen, Computational Materials Science 246, 113388 (2025).

[2] Ngoc Linh Nguyen, The Hung Dang, Tien Lam Pham, and Thi Minh Hoa Nghiem, Journal of Electronic Materials (2025); https://doi.org/10.1007/s11664-025-12066-4

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Presenter: Nguyen Ngoc Linh

O.2 – Oral, VCTP-50

Structure Prediction in the Search for Hydride-Based High-Temperature Superconductors

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Materials scientists have long chased the dream of finding a superconductor that works at room temperature, and this ambition continues to fuel ceaseless experimentation. In the present study, computer-aided crystal-structure prediction identified a novel hydride, YSc2H24, that crystallizes in a hexagonal lattice with space group P6/mmm and survives only under extremely high

pressures. Its arrangement is striking: dual metallic cages, one housing Sc and the other containing Y, nest within the lattice like Russian dolls, lending the material unusual geometric properties. A comprehensive calculation, which projected phonon dispersions, mapped electron-phonon coupling, and solved the isotropic Eliashberg equation, yielded an exceptionally high dimensionless coupling constant, $\lambda = 3.27$, and pinned the critical temperature Tc between 302 and 330 K at roughly 310 GPa. Remarkably, Tc remains above room temperature even as the external pressure increases. Should experimental verification follow, the compound's exceptional Tc and cage-like topology promise fresh insights into the already puzzling physics of high-temperature superconductivity and may open doors to entirely new classes of applications.

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Presenter: Nguyen Duc-Long

O.3 – Oral, VCTP-50

$U(1)_N$ as a common source for light fermionic dark matter and radiative neutrino masses

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Within the framework of a $U(1)_N$ extended Standard Model, we explore mechanisms to simultaneously generate small neutrino masses and keV-scale fermionic dark matter (DM). These include: a radiative seesaw mechanism to produce keV-scale DM candidates and a radiative inverse seesaw mechanism to generate the tiny masses of active neutrinos. The models residual Z_2 symmetry plays a dual role: it ensures DM stability by forbidding its decay and suppresses mixing between DM and active neutrinos, thereby evading stringent astrophysical and cosmological constraints. It is well-established that keV dark matter can be thermally generated during the early stages of the Universe, wherein it decouples while remaining relativistic, facilitated by $U(1)_N$ portal interactions, but it gets overproduced thermally. To reconcile this overabundance with observational limits, we invoke late-time entropy dilution from the decay of long-lived particles, which effectively reduces the DM relic density. Crucially, the proposed parameter space accommodates both observational data of cosmic inflation and kev dark matter, offering a unified resolution to these distinct challenges in particle cosmology.

Presenter: Do Thi Huong

O.4 – Oral, VCTP-50

Refining Gravitational Wave and Collider Physics Dialogue via Singlet Scalar Extension

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Employing effective field theory techniques, we advance computations of thermal parameters that enter predictions for the gravitational wave spectra from first-order electroweak phase transitions. Working with the real-singlet-extended Standard Model, we utilize recent lattice simulations to confirm the existence of first-order phase transitions across the free parameter space. For the first time, we account for several important two-loop corrections in the high-temperature expansion for determining thermal parameters, including the bubble wall velocity in the local thermal equilibrium approximation. We find that the requirement of completing bubble nucleation imposes stringent bounds on the new scalar boson mass. Moreover, the prospects for detection by LISA require first-order phase transitions in a two-step phase transition, which display strong sensitivity to the portal coupling between the Higgs and the singlet. Interestingly, signals from di-Higgs boson production at the HL-LHC probe parameter regions that significantly overlap with the LISA-sensitive region, indicating the possibility of accounting for both signals if detected. Conversely, depending on the mixing angle, a null result for di-Higgs production at the HL-LHC could potentially rule out the model as an explanation for gravitational wave observations.

Presenter: Tran Van Que

O.5 – Oral, VCTP-50

Quantum many-electron simulation: from correlated mean-field to quantum computing

Tran Nguyen Lan

University of Science, VNU-HCM

For quantum many-body problems, it is crucial to have methods that strike a balance between accuracy and computational costs. Quantum computing is an emerging technology that is expected to tackle issues unsolvable by classical computing. Unfortunately, quantum computing is not yet fully practical due to the current limitations of quantum hardware, and the current state of quantum computing is referred to as the noisy intermediate-scale quantum (NISQ) era. Thus, quantum-classical hybrid approaches have been actively developed to bring quantum computing into realistic applications. In this talk, I will first discuss our current work on correlated mean-field theory (CMFT) for many-body problems in both molecules and solids. I will then present our recently developed downfolding framework derived from CMFT to facilitate variational quantum eigensolver (VQE) in quantum simulation of molecules and solids.

Presenter: Tran Nguyen Lan

O.6 – Oral, VCTP-50

Exploring CP Violation and EDM Cancellation in a Scale-Invariant g2HDM

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Recent LHC data indicate that the discovered scalar particle with a mass of 125 GeV closely resembles the predictions of the Standard Model (SM). While the scale of new physics could lie well above the TeV range, current observations do not rule out scenarios in which new particle masses are below the TeV scale, provided their couplings to SM particles are "aligned" to mimic SM-like behavior. Another significant experimental development is the stringent limit on the electron electric dipole moment (EDM), which strongly constrains CP-violating effects in the Higgs sector.

In this talk, we explore a scale-invariant general two-Higgs-doublet model (SI-g2HDM) with explicit CP violation. Using the method of Gildener and Weinberg, we analyze the Higgs mass spectrum and couplings at the one-loop level, focusing on CP violation originating from both the scalar and Yukawa sectors. We demonstrate that tree-level CP mixing vanishes along a flat direction, resulting in SM-like Higgs couplings to gauge bosons and fermions that satisfy current LHC constraints. At the one-loop level, CP violation in the Higgs sector is entirely determined by the additional Yukawa couplings. Furthermore, in the presence of a complex top Yukawa coupling (ρ_{tt}), we find that the electron EDM vanishes when $\arg = n\pi/2$, where n is an integer. This behavior is in sharp contrast to that in the conventional general 2HDM. Time permitting, we will also discuss cases involving a nonzero additional electron Yukawa coupling.

Presenter: Senaha Eibun

O.7 – Oral, VCTP-50

Gravitational-Wave Signatures of the Kozai-Lidov Effect

Lott Peter Tell (1), Nguyen Quynh Lan (1), Li Gongjie (2)

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Gravitational-wave astronomy has provided a unique probe into the dynamics of globular clusters, active galactic nuclei, and few-body gravitationally interacting systems. While binary systems are a prevalent source of gravitational waves in ground-based interferometers, such systems could also be perturbed by the presence of a distant, third body, i.e. a supermassive black hole. Over secular timescales (i.e. timescales larger than the orbital period of the binary), the gravitational interaction of the binary with the third body may lead to orbital resonances. One such resonance, known as the Kozai mechanism, causes an oscillation between the values of the binary's eccentriCity and its inclination with respect to the third body, driving the initially circular binary to arbitrarily high eccentricities at low inclinations. Such eccentricities result in close encounters near periapsis, with GW bursts particularly relevant for ground-based detectors. In this presentation, I focus on the Kozai mechanism in the hierarchical triple body system within the context of gravitational wave astronomy, producing gravitational-wave templates in cases that may be detectable by future detectors, and speculate on the event rate of these kinds of systems.

Presenter: Lott Peter Tell

O.8 – Oral, VCTP-50

Capture, conversion, and utilization of hydrocarbon fuel from carbon dioxide:

A case study

Do Ngoc Son (1,2), Nguyen Thi Xuan Huynh (3), Dang Long Quan (1,2,4), Huynh Tat Thanh (1,2,5), Le Nguyen Bao Thu (1,2), Pham Ngoc Thanh (5), Pham Thanh Hai (1,2,6), Ong Kim Le (1,2,7,8), Tran Phuong Dung (9,10), Phan Thi Hong Hoa (1,2), Nguyen Luu Thanh Ngan (1,2), Nguyen Thi My Ngoc(1,2), Nguyen Vu Dang Khoa (1,2)*

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Using fossil fuels and their derivatives releases a significant amount of CO_2 into the atmosphere, which is a major contributor to the greenhouse effect and global warming. Therefore, reducing CO_2 emissions from energy consumption is crucial to mitigating the negative impacts associated with this gas. Various approaches have been explored, with a sustainable and long-term solution being the adoption of renewable energy sources such as wind, tidal, solar, and hydrogen. Another strategy that has been implemented is the liquefaction of CO_2 for underground storage; however, this method is not economically efficient and also presents safety risks, including potential leaks. A particularly promising approach is the development of a "green energy CO_2 cycle." In this cycle, CO_2 from the atmosphere or from exhaust emissions is converted into hydrocarbon fuels through reactions with water or hydrogen using electrochemical processes or sunlight. The hydrocarbon products of this cycle can also be utilized in proton exchange membrane fuel cells. The use of hydrocarbon products from the carbon cycle does result in CO_2 emissions into the environment; however, overall, it balances out, as the CO_2 released is derived from CO_2 that was previously absorbed. To implement either burial technology or the conversion of CO_2 into fuels, robust support from CO_2 capture technologies is essential, particularly those utilizing adsorption phenomena in solid structures. Materials with exceptionally large surface areas and pores, such as metal-organic frameworks (MOFs), are particularly promising for CO_2 capture due to their advantages as physical adsorbents. MOF-based storage technology offers several benefits over other methods, including rapid storage kinetics and completely reversible storage and desorption processes. As a result, using MOFs for gas capture and storage can lead to cost reductions because of easy desorption and the potential for reusing the MOF material. This report will present a case study from our group, detailing the process of capturing CO_2, converting it into fuel, and utilizing that fuel. This study has been conducted by integrating various tools, including modeling, density functional theory calculations, and experimental methods.

Presenter: Do Ngoc Son

O.9 – Oral, VCTP-50

Tunable Thermal Transport in Hole-Doped Monolayer Penta-Graphene: A First-Principles and Machine Learning Study

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Electron–phonon coupling (EPC) in semiconductors is typically much weaker than phonon–phonon (ph–ph) scattering, and its effect on lattice thermal conductivity (κ_l) is often considered negligible. Here, using first-principles calculations combined with machine learning, we show that in the monolayer penta-graphene, EPC can surpass intrinsic ph-ph scattering under carrier doping. Near the Van Hove singularity, high hole doping levels lead to a fourfold reduction in κ_l at room temperature and suppress its temperature dependence. This anomalous behavior arises from the joint effects of mirror symmetry breaking and weak ph–ph scattering dominated by normal processes. Our results reveal a new mechanism for tuning heat transport in 2D materials via doping-enhanced EPC, offering pathways for thermal management and device engineering.

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Presenter: Vo Khuong Dien

O.10 – Oral, VCTP-50

Theoretical study of a quantum control to create the photon-dressed states using pump lasers

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Recently, we proposed a photo-control scheme based on the dynamic Stark shift mechanism to create the unidirectional coherent angular momentum in low-symmetric aromatic rings [1,2]. However, compared with the coherent angular momentum induced by the circularly polarized (CP) laser in highly symmetric aromatic ring molecules [3,4], the obtained angular momentum intensities are relatively weaker due to a pulse-train shaped form of the angular momentum. Furthermore, in the above studies, different photo-control approaches were applied to aromatics with different symmetries. Meanwhile, we recently highlighted utilizing the helical-photon-dressed states formed by a CP or elliptically polarized (EP) laser [5] to provide more consistent treatment. This study was verified using a minimal three-electronic-state model. The time-dependent

Schrödinger equation was solved within the semi-classical treatment of the light-matter interaction, and rotating wave approximation (RWA) under frozen nuclei condition. We have presented that the two photon-dressed states represent classical rotation; in contrast, the remaining dressed state shows non-classical rotation in low and highly symmetric aromatics. Here, classical rotation means that the unidirectional pi-electron rotation is the same as that of the rotational direction in the rotating electric field determined by the classical equation of motion, whereas non-classical rotation indicates the opposite direction. In the photon-dressed states approach, the dressed states were formed in the presence of the CP or EP laser, however, due to a lack of initial preparation for the dressed states, it is crucial to consider a process for creating the photon-dressed states starting from the ground state using the designed pump lasers. Quantum design of pump lasers is required for dynamical processes to be feasible experimentally. For this purpose, we have analytically designed pump lasers to generate the photon-dressed states in low-symmetric aromatic rings, and show two photo-control approaches using two resonant linearly polarized (LP) lasers, and an EP laser as pump lasers.

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Presenter: Mineo Hirobumi

O.11 – Oral, VCTP-50

Quantum Batteries VS Lithium-ion battery

Nguyen Quang Hung, Nguyen Tuan Loi and Tran Dong Xuan

Researcher and lecturer

This report compares lithium-ion batteries with emerging quantum batteries, highlighting differences in operating principles and potential applications. While lithium-ion batteries base on electrochemical ion transfer and are widely used in modern electronics, quantum batteries exploit quantum phenomena such as tunneling, entanglement, and superposition for ultrafast charging and long-term energy retention. We introduce models using FGMOS transistors, outline the structural design and theoretical advantages of quantum batteries. Recent advancements—including room-temperature demonstrations and photon-assisted charging—are updated. Although still in early development, quantum batteries show strong promise for future use in high-efficiency energy storage systems.

Keywords: Quantum battery, lithium-ion, Electron tunneling.

Presenter: Tran Dong Xuan

O.12 – Oral, VCTP-50

Thermoelectric transport in some charge Kondo circuits: Generalized Cutler-Mott relation

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In this talk, we revisit charge Kondo circuits, focusing on two models: the single-site two-channel model and the two-site two-channel model. We compute the thermopower using the Cutler-Mott formula and compare our results to thermopower values obtained directly as the ratio of the thermoelectric coefficient to the electrical conductance. Based on this comparison, we propose a generalized Cutler-Mott relation that applies to both charge Kondo setups. Remarkably, this generalization holds in both the Fermi liquid and non-Fermi liquid regimes. The additional logarithmic prefactor introduced in our modified relation highlights the role of charge Kondo correlations in thermoelectric transport.

Presenter: Nguyen Thi Kim Thanh

O.13 – Oral, VCTP-50

TDNRG approach to work distributions for quantum impurity systems

H. T. M. Nghiem

Phenikaa University

Work distribution function P(W) for a quantum impurity system at fine temperature is derived within the time-dependent numerical renormalization group (TDNRG) formalism. The precision of WDF is exhibited via the sum-rule and the Crooks relations at an arbitrary temperature. While, at zero temperature, the power law behavior of P(W) is observed as W is closed to the approaches the minimum work. The details will be shown in the presentation.

Presenter: Nghiem Hoa

O.14 – Oral, VCTP-50

Towards a dark grand unification

Phung Van Dong (1), Le Duc Thien (2)

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I show that the trinification encompasses the dark sector of the universe. The trinification gauge symmetry contains a matter parity that assigns the new fields to be odd, while the normal fields to be even. The lightest of the odd fields, either a neutral fermion or a neutral scalar, is stabilized by the matter parity, responsible for dark matter. The odd vector field cannot be a dark matter candidate as ruled out by direct detection experiment. This setup suppresses dangerous flavor-changing neutral currents due to down-type quark mixings naturally by the matter parity. Neutrino masses and phenomenological processes are hinted.

Presenter: Phung Van Dong

O.15 – Oral, VCTP-50

Type-I two Higgs doublet model: current data fitting and future detection ability

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(2) VNU - University of Science;
(3) The High Energy Accelerator Organisation (KEK)

Considering various theoretical and phenomenological constraints, we have found the best-fitted parameter set in the type-I two Higgs doublet model. This optimal parameter set can be tested by precisely analyzing specific decay processes of D^+, B^0, and the light Higgs boson. For a direct search of the model at future colliders, we have proposed an investigation of the $t\bar{t}$ $b\bar{b}$ signal at the ILC to detect the new physics of the model.

Presenter: Tran Minh Hieu

O.16 – Oral, VCTP-50

Dimensional reduction issue of a six-dimensional Kaluza-Klein theory

Tuan Q. Do

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In this talk, we will present a dimensional reduction issue of a six-dimensional Kaluza-Klein theory. In particular, we will show that two approaches of dimensional reduction lead to different four-dimensional effective actions although using the same six-dimensional metric. It is noted that the first dimensional reduction is a direct one, i.e., from six-dimensional spacetimes directly to four-dimensional ones, via a $T^2 \equiv S^1 \times S^1$ compactification. On the other hand, the second dimensional reduction is an indirect one, i.e., from six-dimensional spacetimes to five-dimensional ones then four-dimensional ones, via two separated S^1 compactifications. It could therefore address an important question of which approach is more reliable than the other.

Presenter: Do Quoc Tuan

O.17 – Oral, VCTP-50

Understanding the mechanism of the co-doping effect on ionic conductivity of Gd3+ and M3+ (M = Nd, Pr) co-doped ceria for solid oxide fuel cell applications

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In this work, statistical moment method (SMM) is first developed to illuminate the atomic mechanism of the co-doping effect on improving ionic conductivity of Gd3+ and M3+ (M = Nd, Pr) co-doped ceria (CeO2) electrolytes. The simultaneous existence of co-dopants with the different characters in ionic size and oxygen vacancy trapping effect alters the lattice's local structure, the component interactions between charged defects, and causes the asymmetric profiles with

a reduced energy barrier. These factors work together to minimize the activation energy and provide more transferable oxygen vacancies with high ionic mobility for ionic conduction. The SMM results of dopant-oxygen vacancy binding, migration, and activation energies exhibit as a non-linear function of the co-dopant content. The lower activation energy and higher bulk ionic conductivity of doubly doped ceria compared to singly doped ceria in the low and high temperature regimes demonstrate the synergistic role of co-doping effect. The maximum values of bulk ionic conductivity are found with $Ce0.8Gd0.12Nd0.08O2-\delta$ (σ773K = 6.25 $\times 10^{-3}$ S/cm) and $Ce0.8Gd0.14Pr0.06O2-\delta$ (σ773K = 5.88 $\times 10^{-4}$ S/cm) for a series of co-dopant contents. Our results are completely compared with experiments.

Presenter: Le Thu Lam

O.18 – Oral, VCTP-50

Phase transitions in Hatano–Nelson lattice chains with periodically modulated disorder

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We theoretically study a one-dimensional Hatano–Nelson lattice with mosaic-modulated on-site potentials to uncover the interplay between non-Hermiticity, disorder, and periodicity in shaping spectral and dynamical properties. Through analytical and numerical analyses, we demonstrate that the mosaic modulation generates closed-loop energy trajectories in the complex plane, which coalesce as the imaginary gauge field approaches a critical threshold. Remarkably, the periodic arrangement of disordered potentials enables tunable real–complex spectral transitions and localization–delocalization crossovers at well-defined spectral regions, marked by the emergence of mobility edges. Notably, delocalized states with complex eigenvalues exhibit characteristic nodal structures. To further elucidate the transport behavior, we investigate wave packet dynamics via the mean square displacement and center of mass. Our results reveal an abrupt transition from localization to ballistic spreading induced by the structured disorder—an effect absent in the standard Hatano–Nelson model with weak non-Hermiticity. Our work highlights the rich physics driven by structured disorder in non-Hermitian systems.

Presenter: Nguyen Ba Phi

O.19 – Oral, VCTP-50

First-order magnetic transition and giant magnetic entropy change induced by random anisotropy in external fields

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This study explores first-order magnetic transitions (FOMT) and isothermal first-order magnetization processes (FOMP) in a two-dimensional (2D) spin system through Monte Carlo sim-

ulations applied to the spin-1 Blume-Capel model, incorporating random anisotropy under an external magnetic field. Significant variations in isothermal magnetic entropy are observed near the critical temperature $T_C^{(1)}$ of the FOMT when both the magnitude (D) and probability (p) of the random anisotropy are sufficiently high. The FOMT is characterized not only by an abrupt change in magnetization at $T_C^{(1)}$ but also by shifts in the distributions of energy and magnetization histograms. From these analyses, we construct a phase diagram illustrating the transition from a second-order magnetic transition (SOMT) to a FOMT, driven by random anisotropy, and compare it with previous findings in Ref. [1]. The calculated magnetic entropy change $|\Delta S_M|$ reveals a pronounced magnetocaloric effect near $T_C^{(1)}$, especially when the applied magnetic field approaches the critical threshold h_{cr} associated with the FOMP. Additionally, the entropy change during the FOMT is notably greater than that observed in the SOMT under equivalent low-field conditions. Finally, the temperature-dependent magnetic properties near the FOMT are compared with experimental data from $Cr_{11}Ge_{19}$ samples.

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Presenter: Nguyen Hai Phong

O.20 – Oral, VCTP-50

Numerical Simulation of Black Hole to White Hole Transition Using Entangled Lattice-Based Qubits Formalism

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This study introduces a quantum gravitational simulation of black hole (BH) formation and white hole (WH) emergence using an entangled lattice-based qubits formalism. Spacetime is modeled as a crystalline lattice where each site holds a qubit entangled with its neighbors. We reformulate gravitational curvature in terms of quantum entanglement amplitudes and simulate the transition from BH collapse to WH expansion via a renormalization-free quantum gravitational field equation (QGFE). We implement a dynamic evolution mechanism triggered by curvature saturation, demonstrating a full bounce across the Planck regime. Visualization confirms a smooth entanglement-driven geometry connecting the BH and WH regimes.

Presenter: Srichan Chavis

O.21 – Oral, VCTP-50

Effects of boron or nitrogen dopants on electronic and optical properties of the graphene/h-BN heterostructure

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Two-dimensional (2D) materials have emerged as promising candidates for advanced semiconductor devices due to their unique quantum and surface-dominated properties [1]. Among them, van der Waals heterostructures, formed by stacking atomically thin layers, enable new functionalities beyond those of individual components [2]. The graphene/hexagonal boron nitride (G/h-BN) system combines the excellent conductivity of graphene with the insulating characteristic of h-BN [3,4] to effectively tailor its optical properties [5]. However, the effects of B and N dopants on the optical properties of G/h-BN remain ambiguous. This work performs the first-principles investigation to clarify the problem. The study examines the structural configurations, the stability of various dopant positions, and the corresponding changes in electronic band structures, density of states, and optical absorption and emission characteristics. The findings will offer theoretical guidance for designing tunable 2D materials for nanoelectronic and optoelectronic applications.

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Presenter: Ngân Lưu Thanh Nguyễn

O.22 – Oral, VCTP-50

Multielectron polarization-induced frequency shifts in high-order harmonic generation: a manifestation of molecular asymmetry

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High-order harmonic generation (HHG) from atoms and molecules under intense laser fields has been a useful tool in ultrafast science, often modeled using the single-active-electron (SAE) approximation [1]. This approximation assumes that only the outermost electron responds to the laser field, while inner-shell electrons remain frozen. However, advance experimental evidence has reveals that strong-field behaviors cannot be explained without considering multielectron interactions. One prominent manifestation of multielectron effects is the dynamic polarization of the core electron, commonly referred to as multielectron polarization (MEP) [2]. This effect becomes especially important in targets with large polarizabilities, such as polar molecules. Considering HHG emission, MEP has been shown to influence the emission intensity, and the spectral structure [2-4].

While previous work has focused on MEP-induced modulation of HHG intensity, such as the even-to-odd ratio for polar molecule, i.e. the intensity ratio between the even-order harmonic and the neighboring odd-order harmonic [4], the influence of MEP on the frequency positions of HHG has not been figured out. Given that HHG results from the coherent interference of attosecond bursts generated every half optical cycle, any phase difference between two adjacent bursts—arising from molecular asymmetry or the laser waveform—can shift the resulting harmonic frequencies [5].

In this study, we investigate how MEP induces frequency shifts in HHG spectra from polar molecule driven by few-cycle laser pulses by distorting the phase difference between attosecond bursts. We first present an analytical demonstration to this effect and subsequently validate it through numerical simulations by solving the time-dependent Schrödinger equation (TDSE). Furthermore, we demonstrate the universality of the MEP-induced frequency shift when varying laser parameters. Finally, we indirectly confirm this effect by analyzing available HHG data when adopting multicycle laser pulses.

By investigating the interaction between CO molecules and few-cycle laser pulses, we reveal that MEP causes a significant shift in harmonic peak frequencies, reaching up to 0.8 harmonic orders (equivalent to 1.24 eV) near the cutoff region. This phenomenon is attributed to the MEP-induced asymmetry in the phase difference between two adjacent attosecond bursts. Although direct experimental confirmation is currently limited, we provide indirect validation by connecting measured odd-even intensity ratios with predicted peak shifts. Our results highlight the role of HHG frequency shifts as a spectral feature for characterizing multielectron effects and probing the asymmetry of polar molecules.

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Presenter: Nguyen Huynh Kim Ngan

O.23 – Oral, VCTP-50

Emergence of the Liouvillian Skin Effect in Driven – Dissipative Ultracold Atom Systems

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Topological insulators have been shown to exhibit the Liouvillian skin effect ([1], [2]), whereby dynamically stable edge states with zero energy emerge at the boundaries of the system due to the non-Hermiticity of the Hamiltonian describing the system. The importance of this Liouvillian skin effect manifests itself in, among other things, the relaxation time of dissipative quantum systems [3], whereby it is shown that the relaxation time, or the timescale over which the system achieves its steady state, is inversely proportional to the magnitude of the largest eigenvalue

corresponding to these anomalous zero-energy edge states. We investigate whether this is indeed the case in a driven-dissipative ultracold atom system described in Ref. [4], which consists of a gas of ultracold atoms trapped in an array of harmonic potentials. We show that, under certain conditions, the Liouvillian skin effect will manifest itself in this system, and we derive the explicit form of the eigenvalues corresponding to these anomalous zero – energy edge states that are the hallmark of the Liouvillian skin effect. From this, we then obtain the relaxation time for the system, and compare the calculated relaxation time with the time obtained numerical simulations showing how the system evolves over time to its steady state.

Presenter: Caballar F. Roland Cristopher

O.24 – Oral, VCTP-50

2D rotating Bose-Einstein condensation at the critical rotation speed

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of the Thomas-Fermi functional is to link the emergence of vortex lattices (the Abrikosov problem). When turning from repulsive to attractive interactions, the system is unstable since there is a balance between kinetic and interaction energies. In the regime where the strength of the interaction approaches a critical value from below, the system collapses to a profile obtained from the (unique) optimizer of a Gagliardo-Nirenberg interpolation inequality. This was established before in the case of fixed rotation frequency. We extend the result to rotation frequencies approaching, or even equal to, the critical frequency at which the centrifugal force compensates the trap. We prove that the blow-up scenario is to leading order unaffected by such a strong deconfinement mechanism. In particular, the blow-up profile remains independent of the rotation frequency.

Presenter: Nguyễn Đình Thi

O.25 – Oral, VCTP-50

Possible existence of the pygmy dipole resonance built on excited states

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This report presents recent studies on the formation of the Pygmy Dipole Resonance (PDR) at finite temperatures, i.e., PDR built on excited states. Both experimental and theoretical investigations have confirmed the existence of Pygmy dipole collective oscillations in the low-energy tail of the Giant Dipole Resonance. The findings also reveal isospin mixing at the nuclear surface and indicate a violation of the Brink-Axel hypothesis in the low-energy region.

Presenter: Le Tan Phuc

O.26 – Oral, VCTP-50

On the Leggett-Garg Inequality Testing with Neutrino Oscillation Measurements**

Son Cao

IFIRSE, ICISE

The Leggett-Garg inequality (LGI), known as time-analogue Bell's inequality, provides a framework to test the quantumness of physical systems. This talk is to review and discuss recent developments in applying the LGI to neutrino oscillations, a quantum interference phenomenon driven by the leptonic mixing. The neutrino oscillations measurements offer a compelling avenue for such tests due to their maintained coherence over macroscopic distances. We will propose and examine the LGI test with reactor-based and accelerator-based neutrino oscillation measurements.

Presenter: Cao Van Son

O.27 – Oral, VCTP-50

Thermoelectric properties of penta-InP_5: A first-principles and machine learning study

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High-performance thermoelectric (TE) materials with good mechanical durability are attracting significant interest for applications in smart wearable devices, particularly for harvesting energy from body heat. This study presents a comprehensive analysis of the thermoelectric and mechanical properties of a novel two-dimensional material, monolayer penta-InP_5, using first-principles calculations combined with on-the-fly machine learning potentials (FMLP). Our computational results show that penta-InP_5 exhibits outstanding thermoelectric properties at room temperature (300 K). The material achieves a remarkable figure of merit (ZT) of 0.51 for p-type (hole) doping and 0.42 for n-type (electron) doping. This high performance stems from an optimal combination of high electrical conductivity, a favorable Seebeck coefficient, and a very low lattice thermal conductivity (approximately 1.82 $W{\cdot}m^{-1}{\cdot}K^{-1}$). The low thermal conductivity is attributed to low phonon group velocities and strong lattice anharmonicity. Furthermore, penta-InP_5 demonstrates impressive mechanical properties, with an in-plane stiffness of about 52 N/m and a large ductile fracture strain of up to 23.

Presenter: Lê Nhật Thanh

O.28 – Oral, VCTP-50

Solvation effects on protein folding in a simple lattice model

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The aqueous solvent profoundly influences protein folding, yet its effects are relatively poorly understood. In this study, we investigate the impact of solvation on the folding of lattice proteins by using Monte Carlo simulations. The proteins are modeled as self-avoiding 27-mer chains on a cubic lattice, with compact native states and structure-based Go potentials. Each residue that makes no contact with other residues in a given protein conformation is assigned a solvation energy ϵ_s, representing its full exposure to the solvent. We find that a negative ϵ_s, indicating a favorable solvation, increases the cooperativity of the folding transition by lowering the free energy of the unfolded state, increasing the folding free energy barrier, and narrowing the folding routes. This favorable solvation also significantly improves the correlation between folding rates and the native topology, measured by the relative contact order. It is suggested that the solvation potential in our model is related to the polar interaction between water and peptide groups in the protein backbone.

Presenter: Nguyen Thi Thuy Nhung

O.29 – Oral, VCTP-50

Degenerate points in wetting phase diagram of a dilute ternary Bose-Einstein mixtures

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In the present study, we investigate the wetting phase behavior of a dilute ternary Bose-Einstein condensate mixture at zero temperature within the theoretical framework of the Gross-Pitaevskii formalism, employing the double parabola approximation to model interfacial phenomena. Our analysis reveals that the first-order wetting transition line and the nucleation line associated with three-phase coexistence intersect at a set of degenerate points, which reside in the parameter space defined by the interspecies interaction coupling constants. Furthermore, we systematically examine the locus of these degenerate points within the space of intrinsic atomic parameters, particularly in the regime characterized by strong segregation between two of the components.

Presenter: Nguyen Van Thu

O.30 – Oral, VCTP-50

Assessing the impact of ligand substitution on the optoelectronic properties and electron transport behavior of oligophenylene ethynylene

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We present a comprehensive theoretical investigation into the effects of ligand substitution on the optoelectronic and electron transport properties of oligophenylene ethynylene (OPE) molecular wires, employing density functional theory in conjunction with the non-equilibrium Green's function formalism. We show that functionalization of OPE with electron-withdrawing groups, most notably –NO2, leads to a pronounced narrowing of the HOMO–LUMO energy gap and a substantial redshift in the optical absorption spectrum, indicating enhanced electron affinity and improved photophysical response. The electron transport characteristics are significantly modulated by ligand type; OPE derivatives containing –NO2 and –CN exhibit superior electron conductivity at low bias voltages, while the –NH2-functionalized OPE demonstrates ambipolar transport behavior with balanced charge carrier mobility. The computed triplet excitation energies (ET1) suggest that all substituted OPEs are suitable candidates for red-emitting optoelectronic applications, with derivatives bearing –NH2, –Cl, and –CN ligands exhibiting enhanced photoluminescence efficiency due to favorable charge recombination profiles. These findings establish a direct correlation between ligand identity and electronic function, offering design principles for tailoring the performance of π-conjugated molecular semiconductors in nanoelectronic and optoelectronic applications.

Presenter: Nguyen Thi Bao Trang

O.31 – Oral, VCTP-50

Investigating the Talbot effect in binary waveguide arrays

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Waveguide arrays (WAs) are a candidate for studying many classic photonic phenomena, such as discrete diffraction [1], discrete solitons [2], and the generation of diffractive resonant radiation from discrete solitons [3]. Klein tunneling (KT) has also been investigated in BWAs both theoretically [4] and experimentally [5], and was predicted by O. Klein in 1929 [6]. According to Klein, relativistic fermions can tunnel through large repulsive potential steps, higher than the particle's energy, without the exponential decay expected in quantum nonrelativistic tunneling processes governed by the well-known Schrödinger equation [6]. This phenomenon is due to the existence of negative-energy solutions of the Dirac equation [7]. We simulated the Talbot effect by launching a Dirac soliton in binary waveguide arrays [8]. In this talk, we demonstrate that the analytical transmission coefficient in the discrete model with BWAs is in strikingly perfect

agreement with the simulation-based results.

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Presenter: Trần Công Minh

O.32 – Oral, VCTP-50

The Stark effect calculations in spherical coordinates

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The methods for calculating the real or complex eigenenergies and the corresponding eigenfunctions of a hydrogen-like atom with one electron in a uniform electric field directed along the third axis of the Cartesian coordinate system, the Stark effect, are presented. A two-dimensional boundary value problem in partial derivatives in a spherical coordinate system for a fixed magnetic quantum number is solved by the Kantorovich method, which is a reduction in a system of second-order ODEs in the radial variable using the expansion of the desired solution in the basis of angular functions that depend on the radial variable of the ODE as a parameter. The presented method is implemented as algorithms and programs in the Maple system for calculating a set of parametric angular eigenfunctions and eigenvalues, and effective potentials of the ODE system in the radial variable. Estimates of the complex eigenvalues of the energy of the lower part of the Stark effect spectrum are obtained by solving a finite number of equations of the ODE system in the radial variable using the KANTBP 5M program, which implements the finite element method (FEM) in the Maple system.

Presenter: Luong Le Hai

O.33 – Oral, VCTP-50

On Rydberg excitons in two-dimensional semiconductors

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Over the past decade, Rydberg excitons in 2D semiconductors have attracted much attention for potential applications in quantum technologies. Here, we study Rydberg excitons in monolayer transition-metal dichalcogenide (TMD) semiconductors. We determine exciton binding energies and sizes in monolayer TMDs by using the variational method, and show the influences of the surrounding dielectric environment on the exciton properties.

Presenter: Nguyen-Truong T. Hieu

O.34 – Oral, VCTP-50

Spin filtering in ring conductors by electromagnetic dressing

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Transport of ballistic electrons through a 1D-dimensional quantum ring (subjected to Rashba spin—orbit interaction), connected with two external leads, is studied in the presence of external fields. These fields include the optical radiation, produced by an off-resonant high-frequency electric field, and a perpendicular magnetic field. With the aid of the Floquet theory, the key role of the interplay between the optical radiation intensity and the Rashba interaction is established for spin filtering effect of an initially arbitrary polarized electron beam at zero and low magnetic fields.

Presenter: Nguyen Danh Tung

O.35 – Oral, VCTP-50

Machine learning enhanced global optimization and its application in elucidating hydrogen insertion in $SrMO_y$ (M = Fe and Co)

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Hydrogen insertion/extraction can induce topotactic phase transitions, significantly altering the structural and electronic properties of Fe and Co-based-transition metal oxides, $SrMO_y$ (M = Fe, Co). These reversible transitions are of great interest for applications in resistive switching memory, and tunable electronic/ionic conductors for energy conversion and storage systems. Despite

their promise, a comprehensive understanding of the phase transition behavior of $SrMO_y$ remains elusive, largely due to complex potential energy landscapes. Herein, we apply the machine learning-enhanced global optimization (GOFEE) method1,2 to investigate hydrogen insertion behavior in $SrMO_y$. By combining evolutionary algorithm (EA) search with a Gaussian Process Regression (GPR) surrogate model, we efficiently identify stable hydrogenated phases of $SrMO_y$ and elucidate thermodynamic stability of $SrMO_y$ under varying hydrogen and oxygen chemical potentials.3,4 First-principles calculations are used to analyze the structural transformations, energetics, and electronic properties of the predicted phases. To validate the computational models, we characterized protonated $SrCoO_{2.5}$ epitaxial films using photoelectron holography.5 Changes in holography patterns upon protonation, caused by cation displacements, were well reproduced by simulations based on GOFEE predicted structures. This confirms the effectiveness of combining advanced modeling and experimental characterization to elucidate H insertion to SrMOy.

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Presenter: Pham Ngoc Thanh

P.1 – Poster, VCTP-50

Impact of Channel Asymmetry on Thermoelectric Transport in a Two-Channel Charge Kondo System

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We theoretically revisit an asymmetric two-channel charge Kondo model, previously studied in Phys. Rev. B 82, 113306 (2010), in the context of its experimental realization reported in Z. Iftikhar et al., Nature (London) 526, 233 (2015). The nano-device under consideration consists of a large metallic quantum dot embedded in a two-dimensional electron gas (2DEG), strongly coupled to two electrodes via nearly transparent single-mode quantum point contacts (QPCs). The 2DEG is in the integer quantum Hall regime, with asymmetric reflection amplitudes at the QPCs. We find that the thermopower and figure of merit are reduced by the channel asymmetry, while the Kondo resonance width and the Lorenz number near the Coulomb peak are enhanced. Finally, we propose a method to improve the thermoelectric efficiency of the device.

Presenter: Nguyen Hong Quang

P.2 – Poster, VCTP-50

Stochastic generation of magnetization in the one-dimensional Ising model exposed to Gaussian white, Brownian red, and pink noises

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To project to a particular final state, stochastic resetting is a useful tool among lattice systems. At the same time, as fluctuations of physical properties are observable among experiments, perturbing toy models with noise subjected to noise provide more insights into experimental results observed in laboratories. In this study, simulations involving a one-dimensional Ising spin chain subject with reset probability and particular kinds of noise are performed. Perturbing the lattice with a Brownian red noise exhibits plateaus of magnetization in certain time intervals at fixed temperatures compared to that of the Gaussian white noise. However, both kinds of noise exhibit random fluctuations of magnetization as functions of temperature. A smoother downward trend as the temperature increases is exhibited when the lattice is exposed to pink noise. Progress in this line of research can lead to applications ranging from understanding of material properties to biological and medical phenomena such as in epidemiology.

Presenter: Villegas Paat Vladimir

P.3 – Poster, VCTP-50

Molecular Simulation-Assisted Aptamer Selection for Lipopolysaccharide Detection and Development of a Simple Electrochemical Aptasensor

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Lipopolysaccharides (LPS), key components of the outer membrane of Gram-negative bacteria, play a crucial role in bacterial pathogenicity and can trigger severe immune responses, leading to sepsis, endotoxic shock, and other inflammatory diseases. Rapid and accurate LPS detection is essential for diagnosing bacterial infections, monitoring pharmaceutical contamination, and ensuring food safety. Aptamer-based detection offers a promising alternative to traditional methods, providing enhanced sensitivity, specificity, and cost-effectiveness. Recent advances in molecular simulations have further improved aptamer selection by complementing the conventional Systematic Evolution of Ligands by Exponential Enrichment (SELEX) process, allowing for the identification of aptamers with high binding affinity and specificity. In this study, we combined conventional aptamer selection with computational studies to generate a single-stranded DNA (ssDNA) aptamer with high affinity and selectivity for LPS detection. To translate this aptamer into a practical sensing platform, we developed a simple electrochemical biosensor utilizing a biotin-labeled aptamer as the detection probe. Our results demonstrated that this aptamer-based biosensor provides a rapid, highly sensitive, and cost-effective method for LPS detection, making it a promising tool for real-time endotoxin monitoring in biomedical and environmental

applications.

Presenter: Nguyen Hai Ly

P.4 – Poster, VCTP-50

Density Functional Theory Analysis of CH_4 and Its Halogenated Derivatives Adsorption Behavior on SnPb Surface for the Development of Gas Sensors

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In this study, density functional theory (DFT) calculations were performed to explore the adsorption behavior of methane (CH_4) and its chlorinated derivatives—carbon tetrachloride (CCl_4) and methylene chloride (CH_2Cl_2)—on an armchair-edged monolayer SnPb nanoribbon. A comprehensive analysis involving adsorption energies, charge density differences, electronic density of states (DOS/PDOS), band structures (BAND), and induced magnetic moments was conducted to elucidate the interaction mechanisms between these gas molecules and the SnPb surface. The results indicate that while all three species exhibit weak physisorption, the chlorinated molecules display pronounced charge redistribution and orbital hybridization effects in comparison to CH_4. Remarkably, CH_2Cl_2 adsorption induces a spin-polarized state, generating a local magnetic moment of approximately 2.4 μB, suggesting its capacity to modulate the magnetic response of the substrate. Despite these interactions, the SnPb nanoribbon retains its semiconducting character with a stable bandgap of around 0.2 eV, demonstrating considerable structural and electronic stability. These findings offer valuable insights into the microscopic adsorption mechanisms of volatile organic compounds on low-dimensional intermetallic systems and identify SnPb nanoribbons as promising candidates for selective gas sensing applications. The theoretical framework established here can be extended to investigate thermal effects, defect-mediated sensitivity, and environmental stability in the future design of nanoscale sensing materials.

Presenter: Tung Thanh Nguyen

P.5 – Poster, VCTP-50

Metal-insulator transitions in the two-dimensional ionic Hubbard model within coherent potential approximation.

Nguyen Thi Hai Yen, Hoang Anh Tuan

Institute of Physics

We employ the coherent potential approximation to investigate the phase diagram of the ionic Hubbard model on the square lattice. The results show the existence of two insulating phases: a band insulator in the region of large ionic potential Δ and small Coulomb interaction U, and a Mott insulator in the regime of large U. Between these two insulating phases, a metallic phase emerges as an intermediate state. The obtained phase diagram is compared with those on the Bethe lattice.

Presenter: Nguyen Yen

P.6 – Poster, VCTP-50

Electromagnetically Induced Transparency in GaAs/InAs Quantum Wells under Magnetic Field and Phonon Interaction

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We theoretically investigate the absorption properties of a ladder-type three-level system exhibiting electromagnetically induced transparency (EIT) in GaAs/InAs/GaAs semiconductor quantum wells. Using the density matrix formalism in the steady-state regime, we derive an analytical expression for the probe transition coherence under the influence of a coupling laser field, an external magnetic field, and longitudinal optical (LO) phonon interaction. The applied magnetic field induces Landau level quantization, which modifies the transition energies and shifts the EIT window. Meanwhile, the interaction between electrons and LO phonons is modeled as a temperature-dependent broadening mechanism that affects the coherence decay rates and reduces the transparency effect at higher temperatures. Numerical calculations of the probe absorption spectra reveal the interplay between magnetic-field-induced level shifts and phonon-induced spectral broadening. Our results show that the position, depth, and width of the EIT window can be effectively controlled by tuning the magnetic field strength, temperature, and coupling field intensity. This study provides useful insights into coherent light–matter interaction in low-dimensional semiconductor structures and suggests potential applications in photonic switching, optical sensing, and quantum information processing.

Presenter: Tran Cong Phong

P.7 – Poster, VCTP-50

Tracking Diamond Tool Wear in Iron Machining with Machine Learning Simulation Study

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Diamond tools are widely used in ultra-precision machining due to their exceptional hardness and ability to produce high-quality surface finishes. However, when machining ferrous metals like iron, diamond suffers rapid wear, mainly due to complex thermo-chemical reactions at the Fe–C interface. To explore these atomic-scale wear mechanisms, we employed machine learning molecular dynamics (ML-MD) simulations. Our interatomic potential was trained on a dataset of around 6,000 structural configurations and achieved high accuracy, with root-mean-square errors of 130 meV/angstrom for forces and 4 meV/atom for energies. The model accurately reproduces structural and energetic properties of pure bcc iron, carbon, and Fe–C systems. We conducted large-scale cutting simulations involving over 8,000 atoms with 1 fs timesteps over nanosecond durations. Results show that using the diamond surface as the clearance face leads to significantly higher wear than when used as the rake face. Lower cutting temperatures were

found to reduce wear rates. Among the diamond surfaces tested, diamond(111) showed the highest wear resistance. Despite initially predicting wear rates 2–3 orders of magnitude above experimental values, the results are expected to converge with longer simulation times. This study demonstrates the value of ML-MD in revealing wear mechanisms and guiding tool design in ferrous machining.

Presenter: Nguyen Trinh Bao Anh

P.8 – Poster, VCTP-50

Theoretical elucidation of local atomic structures and colossal permittivity properties of Nb-doped TiO_2

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Recently, materials with colossal permittivity (CP) have attracted significant interest due to their potential applications in device miniaturization and high-energy-density storage. To date, CP-based capacitors have primarily relied on materials such as $BaTiO_3$, $CaCu_3Ti_4O_12$ (CCTO), $La_{2-x}Sr_xNiO_4$ (LSNO). However, $BaTiO_3$ exhibits temperature-sensitive permittivity, while CCTO and LSNO suffer from high dielectric loss [1-3]. Achieving both CP and low dielectric loss in a single material remain a significant challenge. TiO_2 doped with pentavalent element (V, Nb, Ta) material has emerged as a promising alternative [4]. Experimental studies have shown that at high temperatures, its CP is primarily attributed to the Maxwell-Wagner-Sillars effect, where electrons accumulate at grain boundaries, leading to a large dielectric dipole. However, at low temperatures, even though the Maxwell-Wagner-Sillars effect is suppressed, the permittivity of doped TiO_2 remains very high (about four-fold compared to the undoped case) [5]. Therefore, the underlying mechanism responsible for the high permittivity at this regime remains unclear. In this study, we investigate the mechanisms underlying the high permittivity of Nb-doped TiO_2 at low temperatures using Density Functional Theory (DFT). Pentavalent ions such as Nb have an additional electron in their outer shell compared to Ti atoms. When Ti is substituted by Nb in TiO_2, this excess electron becomes localized, inducing the local lattice distortion and forming a quasi-particle called polaron. Our DFT results show that the excess electron localizes on a Ti atom neighboring the Nb-dopant, forming a molecular polaron configuration. The energy barrier for polaron hopping between adjacent Ti sites of Nb atom is relatively small (about 20 meV), which allows for flip-flop motion of the molecular polaron even at low temperatures. This hopping process contributes to the formation of large dielectric dipoles, leading to the manifestation of colossal permittivity. Furthermore, when compressive (tensile) pressure is applied to Nb-doped TiO_2, our DFT calculations reveal a decrease (increase) in the polaron hopping barrier. This observation highlights the role of external pressure in modulating the local structure and the permittivity of Nb-doped TiO_2, providing insight into their pressure-dependent behavior.

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Presenter: Dinh Ngoc Dung

P.9 – Poster, VCTP-50

Monte Carlo Simulation of Magnetocaloric Effects in Doped Perovskites

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Monte Carlo simulations are performed to study the magnetic behavior of doped perovskite compounds. The model includes both superexchange and double exchange interactions as pairwise exchange terms, along with an additional multi-spin interaction. With the aim of developing magnetocaloric materials that exhibit strong effects over a broad temperature range near room temperature, recent research has focused on doping as an effective strategy to modify magnetic interactions and phase transition behavior. We investigate how doping influences the phase transition temperature and analyze the system's response to external magnetic fields at various doping levels. Energy histogram analysis is used to examine the characteristics of the phase transition. The magnetic entropy and relative cooling power are determined. The results show good agreement with experimental observations, highlighting the potential of these materials for magnetic refrigeration applications.

Presenter: Nguyen Thi Phuong Thuy

P.10 – Poster, VCTP-50

In silico ion-gated targeting treatment of selected diseases using a stochastically-reset Ising model

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Experiments have shown that vision can be "restored" in blind retinal neurons by stimulating electrical impulses through the embedding of organic semiconductors, which are safe nonionizing implants functioning at body temperature. Furthermore, progress in medicine has shown that targeting cellular ion-gated channels is helpful in treating cancer. Through simulations, this study demonstrates both medical phenomena by factoring in stochastic resetting in a two-dimensional Ising model. Numerical results show that stochastic resetting helps in reducing the average percentage of blind retinal loci through time and increases linearly with respect to its initial value. On the other hand, combining the stochastically-reset Ising model with Hill-like binding curves demonstrates cancer apoptosis by inhibiting ion-gated channels through ligand binding. Progress in this computational study can lead to advances in retinal prostheses and cancer treatment.

Presenter: Lamento-Villegas Barbarona Em-Em

P.11 – Poster, VCTP-50

Boundary Effects and Symmetry Breaking in Maxwell–Chern–Simons Theory

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We investigate the Maxwell–Chern–Simons (MCS) theory in (2+1)-dimensional spacetime confined within a rotating finite disk. Starting from a review of electrodynamics in lower dimensions, we formulate the field equations incorporating both the Chern–Simons term and the effects of rotation. Imposing boundary conditions that enforce the vanishing of the magnetic field at the edge of the disk, we obtain a discrete energy spectrum, effectively quantizing the system. Our analysis reveals that the quantized energy levels are sensitive to both the topological mass and the angular velocity of the system. In particular, the spectra exhibit a marked asymmetry under the reversal of the rotation direction, a direct manifestation of the parity-violating nature of the Chern–Simons term. These findings demonstrate a nontrivial interplay between topological field theory and rotational dynamics, suggesting a broader class of physical systems where topology and geometry together govern spectral properties. Our results extend previous studies on topological mass generation in static backgrounds and provide new insight into parity asymmetry in rotating gauge systems.

Presenter: Nguyen Huu Ha

P.12 – Poster, VCTP-50

The universe as a Grand computational System

Matthew Stanley Leibel

NA

The Grand Computational System proposes a unifying framework in which mass, gravity, time, and consciousness emerge from a quantum information processing substrate. Rather than treating spacetime as a static background and mass as intrinsic, this model views the universe as a dynamic computational engine, where energy is processed through entropy-driven interactions and encoded into spacetime via structured photonic emissions. Spacetime processes information, it is a 2D holographic (reflective) Surface (Boundary) which is also known as the observer itself. Consciousness arises from the self reflection of projecting reality. Key to this theory is an observer-based correction to the Bekenstein Bound, asserting that information is encoded only across the observer-accessible plane, not the full 2D boundary. A case study using a 1 kg steel cube introduces a square root correction to photon emission data, allowing a derivation of Einstein's equation ($E = mc^2$) [Einstein, 1905] from quantum information principles and thermodynamics. Mass is reconceptualized as structured light, and inertia as resistance to information restructuring. Gravity emerges not as a force, but as a computational constraint that adjusts spacetime curvature to optimize information flow. Black holes are framed as nodes of information restructuring, resolving the information paradox by treating Hawking radiation as an encoded, non-thermal emission. Time arises from quantum update cycles, and its directionality is tied to entropy accumulation. Consciousness is modeled as a non-local interaction between the brain and the quantum information field, with subjective experience emerging from entangled informational states. The theory unifies classical and relativistic physics through information and entropy, offering testable predictions in quantum computing, gravitational anomalies, and consciousness studies. In essence, this framework recasts reality as a holographic, self-regulating quantum information system governed by entropy, light, and observation.

Presenter: Matthew Stanley Leibel

P.13 – Poster, VCTP-50

TThe nernst coefficient in semi-parabolic plus semi-inverse squared quantum wells under the influence of intense electromagnetic waves

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This work provides new insight into the quantum Nernst effect (QNE) by establishing a quantitative connection between resonance peak positions and the magneto-phonon-photon resonance condition in semi-parabolic plus semi-inverse squared quantum wells (SPSSQWs) under intense electromagnetic wave (EMW) radiation. In contrast to previous theoretical studies focused on other low-dimensional systems, our results demonstrate the emergence of multi-mode quantum resonances that are characteristic of asymmetric SPSSQW confinement, as well as a refined framework for the precise tuning of magneto-thermoelectric responses in engineered low-dimensional systems. To achieve these results, we use quantum kinetic theory to derive analytic expressions for the Nernst coefficient by calculating the electric conductivity tensors and thermodynamic tensors. Our numerical results for GaAs/AlGaAs SPSSQWs reveal pronounced features in the Nernst coefficient as functions of the EMW frequency, magnetic field strength, confinement frequency, and temperature. Notably, the precise positions of these resonance peaks are calculated by using the magneto-phonon-photon resonance condition. We also observe the shifting towards the higher frequency and amplitude enhancements of the resonance peaks with increasing magnetic field, confinement frequency, EMW frequency, while changes in temperature do not affect the positions of the resonance peaks. Our results establish a robust theoretical foundation for the controlled manipulation of thermomagnetic transport in SPSSQWs, paving the way for future experimental validation and device applications.

Presenter: Nguyen Quang Son

P.14 – Poster, VCTP-50

The transfer of quantum entanglement in a rhombic spins system

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We consider the model of a rhombic spin system that consists of four spins. In the model, the spins are coupled with each other by inner and outer Ising interactions. We show that, in the considered system, quantum entanglement can be perfectly transferred from a pair of spins to another one. Besides, we also point out that the quality of transferring is not only dependent on the strength of couplings but also on the kind of the transferred quantum entangled state. Furthermore, the appearance of the inner interaction induces the transfer of entangled states selectively depending on the transferring direction.

Presenter: Le Duc Vinh

P.15 – Poster, VCTP-50

Many-Body Effects and Velocity Renormalization in Doped Monolayer MoS_2

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We study electron-electron interactions in doped monolayer MoS_2 using a massless Dirac model and random phase approximation with a modified Keldysh potential. Our results predict many-body effects on the spectral function, quasiparticle dispersion, and velocity at zero and finite temperatures, considering carrier density, electric field, and spin polarization. We find strong many-body signatures and spectral instabilities at low densities and small wave vectors. The velocity renormalization shows a linear temperature correction and complex temperature dependence, with notable differences between on-shell and Dyson self-energy approaches.

Presenter: Le Van Tan

P.16 – Poster, VCTP-50

Tuning electronic and magnetic properties of semiconducting silicon carbide nanoribbons using hydrogen doping: A first-principles investigation

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One-dimensional (1D) silicon carbide nanoribbons (SiCNRs) arranging in planar hexagonal lattice, are emerging as potential 1D semiconducting materials owing to their tunable physical properties and unique hybridization characteristics. Using the first-principles calculations, we have systematically explored the rich effects of hydrogen adsorption at various concentrations and distributions on the structural, electronic, and magnetic properties of silicon carbide nanoribbons with armchair and zigzag edge shapes (ASiCNRs and ZSiCNRs). The hydrogen adsorptions result in the stable buckled 1D structures, whereas a transition toward sp^3-like hybridization is occured. The pristine ASiCNRs exhibit as nonmagnetic semiconductor with a direct bandgap of 2.34 eV that becomes ferromagnetic semiconductors with diverse bandgaps and magnetic moments ranging from 1 to 7 μB under various hydrogen adsorptions. Meanwhile, the pristine ZSiCNRs behaves as ferromagnetic semiconductor with spin-splitting bandgap and small magnetic moment that is enhanced under various hydrogenations. The key mechanisms are explored through comprehensive density functional theory (DFT) quantities, including spin-spliting 1D electronic band structures, orbital- and spin-decomposed density of states (DOSs), spin density distribution, and charge density distributions. These findings evidence the highly potential of hydrogenated SiCNRs as versatile 1D materials for future electronic, optoelectronic, and spintronic applications. Keywords: DFT calculations, silicon carbide nanoribbons, armachair and zigzag edges, hydrogen adsorptions, one-dimensional electronic structures, ferromagnetic semi-

conductors.

Presenter: Dang Phuc Dam

P.17 – Poster, VCTP-50

Diverse electronic and magnetic properties of silicon-doped graphene nanoribbons: A hybrid functional study

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In this work, using spin-polarized density functional theory (DFT) calculations with HSE06 hybrid functional, the structural, electronic, and magnetic properties of silicon (Si)-doped armchair and zigzag graphene nanoribbons (AGNRs and ZGNRs) are fully revealed. Pristine AGNRs belong to a nonmagnetic semiconductor with a direct bandgap of 1.92 eV. Under various Si substitutions, nonmagnetic bandgaps are tuned at 1.87, 1.84, 1.45, 1.71, 1.05, and 3.0 eV in the single Si edge-, single Si non-edge-, double Si ortho-, double Si meta-, double Si para-, and 100% Si-substituted AGNR configurations, respectively. Meanwhile, pristine ZGNRs displayed antiferromagnetic semiconducting behavior with a spin degenerate bandgap of 0.81 eV and becomes a ferromagnetic semimetal in the single Si configurations or an unusual ferromagnetic semiconductor in the 100% Si configuration. Under the developed DFT theoretical framework, the formation of quasi π (C-2pz and Si-3pz) and quasi σ (C-2s, C-2pxy and Si-3s and Si-3pxy) bands are identified in the Si-substituted configurations. These quasi π and quasi σ bands show weak separation, resulting in weak quasi sp2 hybridization in Si-C bonds, in which the identified hybridization mechanism are a strong evidence for the formation of stable planar 1D structures in the Si-substituted configurations. Our complete revelation of the essential properties of Si-substituted GNRs can provide a full understanding of their chemically doped 1D materials for various practical applications.

Presenter: Nguyen Duy Khanh

P.18 – Poster, VCTP-50

Electrochemical performance study of a full-cell Lithium-ion battery using a Bi2O3@NaBi(MoO4)2 anode and LiCoO2 cathode

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In this study, LiCoO2 (LCO) material was successfully synthesized in two steps including the fabrication of Co(OH)2 using CoCl2 and NaOH precursors, followed by high-temperature cal-

cination of LiOH and Co(OH)2 synthesized material. X-ray diffraction and scanning electron microscopy were used to evaluate the properties of the synthesized material. The LiCoO2 phase was demonstrated to be present in the LCO material, with a polygonal plate shape of several hundred nanometers in size and tens of nanometers in thickness. When used as a cathode material in lithium-ion batteries, this material exhibited impressive first-cycle capacity, with discharge and charge specific capacities of 122.2 and 140.2 mAh g-1 at 0.2 C, respectively. After 100 cycles, the LCO electrode maintained about 47.8% of the discharge capacity value compared to the first cycle. To demonstrate the feasibility of a full-cell configuration, the synthesized LCO cathode was paired with a Bi2O3@NaBi(MoO4)2 anode. This full-cell system exhibited promising electrochemical behavior, including stable cycling performance and high-rate capacity, indicating its potential application in advanced lithium-ion battery systems.

Presenter: Nguyen Tuan Loi

P.19 – Poster, VCTP-50

Study of the thermodynamic properties of SrZrO3 perovskite by the statistical moment method

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We investigate the thermodynamic properties of cubic- structure SrZrO3 perovskite using the statistical moment method (SMM). The closed analytic expresssion of the potential energy is obtained within approximation up to the fourth-order of the power moments of the atomic displacements and the analytic expressions of the thermodynamic quantities, such as the free energy, thermal expansion coefficients, and heat capacity at the constant volume and constant pressure of SrZrO3 are also derived. Using the suitable potential with patial charge, the numerical results of the thermodynamic quantities of SrZrO3 by the statistical moment method at various temperatures and pressures are obtained and compared with the other theoretical and experimental data. SMM is a good potential to investigate continually the thermodynamic properties of the other perovskite materials with the cubic structure.

Presenter: Cao Huy Phuong

P.20 – Poster, VCTP-50

Nghiên cứu dự đoán cấu trúc Janus hai chiều SnSO và ảnh hưởng của pha tạp kim loại chuyển tiếp lên các tính chất điện tử và từ tính của nó

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Trong những năm gần đây, cấu trúc Janus hai chiều (2D) đã nhận được sự quan tâm đặc biệt nhờ vào các tính chất hấp dẫn đã được chứng minh cả qua thực nghiệm và lý thuyết. Trong nghiên cứu này, chúng tôi dự đoán sự hình thành của cấu trúc Janus SnSO thông qua việc oxy

hóa đơn lớp SnS2. Ảnh hưởng của nồng độ oxy lên cấu trúc và các tính chất điện tử được nghiên cứu một cách đầy đủ. Các kết quả cho thấy hằng số mạng giảm gần như tuyến tính khi tăng dần nồng độ oxy. Ngoài ra, các tính toán cấu trúc vùng năng lượng cho thấy sự thay đổi đáng kể của độ rộng vùng cấm cũng như việc chuyển từ khe trực tiếp sang khe gián tiếp, và ngược lại. Sau khi được chứng minh có độ bền tốt, chúng tôi nghiên cứu ảnh hưởng của pha tạp kim loại chuyển tiếp (V, Cr, Mn và Fe) lên các tính chất điện tử và từ tính của đơn lớp Janus SnSO. Các kết quả thu được chứng minh rằng pha tạp kim loại chuyển tạo nên từ tính đáng kể trong cấu trúc 2D này, ngoài ra các tính chất điện tử giàu đặc tính như bán dẫn từ hay bán kim loại cũng được khẳng định thông qua tính toán cấu trúc vùng năng lượng. Nghiên cứu này chỉ ra khả năng hình thành cấu trúc Janus SnSO từ đơn lớp SnS2 và giới thiệu phương pháp hiệu quả để tạo ra những tính chất mới trong nó hướng đến mở rộng ứng dụng trong thực tế.

Presenter: Do Minh Hoat

P.21 – Poster, VCTP-50

The breaking of $\mu-\tau$ reflection symmetry in a $B-L$ model with $(Z_2\times Z_4)\rtimes Z_2\,(II)$ symmetry

V. V. Vien

Tay Nguyen University

We present a neutrino mass model based on non-Abelian discrete symmetry $(Z_2 \times Z_4) \rtimes Z_2\,(\mathrm{II})$ which successfully accounts for the observed neutrino oscillation data. The atmospheric mixing angle is predicted to be in the higher octant with $\theta_{23}^{(\circ)} \in (47.80,\, 49.40)$ and the predicted range of Dirac CP phase belongs to the lower half plane with $\delta_{CP}^{(\circ)} \in (273,\, 358)$. The hierarchy of lepton masses is naturally achieved and the constraints on the effective neutrino mass is consistent with the recent experimental limits.

Presenter: Vo Van Vien

P.22 – Poster, VCTP-50

Electronic phase diagram of the half-filled ionic Hubbard model on the honeycomb lattice

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The quantum phase transitions of the half-filled ionic Hubbard model on the honeycomb lattice are studied using the coherent potential approximation. The phase diagram of the honeycomb lattice is compared with those of the square lattice. Our results are in good agreement with those obtained via the dynamical mean field theory.

Presenter: Hoang Anh-Tuan

P.23 – Poster, VCTP-50

Optical Force Modulation on Monolayer Graphene in Microcavities: Graphene as a Medium vs. an Interface

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In this study, we investigate the optical force exerted on a graphene sheet positioned within an optical microcavity [1]. The optical conductivity of monolayer graphene is modeled using the Kubo formalism. When graphene is treated as a medium layer, its dielectric response is also considered. Notably, the distinction between modeling graphene as an interface versus as an embedded layer has a significant effect on the magnitude of the optical force and the distribution of the electromagnetic field within the cavity. Our results show that the optical force can increase by nearly a factor of three when graphene is treated as a dielectric medium, compared to when it is considered as an interface [2]. Furthermore, the optical force can also be manipulated by varying the graphene's position within the cavity and the cavity length. These findings not only advance the understanding of light–matter interaction in hybrid photonic systems but also provide valuable guidance for optimizing the design and performance of graphene-based optical devices.

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Presenter: Le Tri Dat

P.24 – Poster, VCTP-50

Two dimensional Semi-Parabolic Plus Semi-Inverse Squared Quantum Well: Theoretical study of the oscillation in the quantum Ettingshausen effect at low temperature under the influence of intense electromagnetic waves.

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The quantum Ettingshausen effect in a Semi-Parabolic Plus Semi-Inverse Squared Quantum Well (SPSSQW) under the influence of intense electromagnetic waves (EMWs) is theoretically investigated using the quantum kinetic equation approach. In this study, we focus on the regime of low temperatures where electron–acoustic phonon scattering dominates the transport processes. The analytical expressions for the Ettingshausen coefficient (EC) are derived, elucidating its dependence on the key physical parameters such as the magnetic field (B), the temperature (T), the intense electromagnetic wave (EMW) frequency, and the SPSSQW confinement frequency. The numerical results reveal that the EC exhibits pronounced quantum oscillations as a function

of the magnetic field, characteristic of Shubnikov–de Haas-type behavior, with the oscillation amplitude decreasing rapidly at the elevated temperatures. Moreover, under the intense EMW irradiation, the resonance peaks emerge in the EC due to the magneto–phonon resonance, and the positions of these peaks can be quantitatively determined from the magneto–phonon resonance condition. Notably, the resonance peak positions remain unchanged with variations in temperature, but display a shift toward the higher frequencies as the magnetic field strength, the intense EMW frequency, and the confinement frequency of the quantum well increase. In addition, the EC is strongly suppressed with increasing temperature, consistent with the thermal broadening of the electron distribution. These findings provide the comprehensive insights into the quantum Ettingshausen effect with the electron-acoustic phonon scattering, and the intense EMW's effects on the magneto-thermoelectric properties of low-dimensional semiconductor systems.

Presenter: Nguyen Dinh Nam

P.25 – Poster, VCTP-50

Size and shape effects on electronic properties of CdX (X=Te, Se, and S) semiconductor nanoparticles

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In this work, we present a theoretical investigation of the size and shape effects on the band gap, conduction-band minimum, and valence-band maximum of semiconductor nanoparticles based on the bond energy model. Analytical expressions are formulated to describe these electronic properties as functions of nanoparticle size and shape. Numerical computations are performed for CdTe, CdSe, and CdS nanoparticles with sizes up to 20 nm. Theoretical results are validated through comparisons with experimental data, demonstrating strong agreement. Our findings reveal a significant widening of the band gap as particle size decreases, particularly for sizes below 5 nm. For larger nanoparticles, the band gap gradually converges toward the bulk semiconductor limit. Our findings enhance the fundamental understanding of the nanoscale electronic properties of CdX (X=Se,Te,S) semiconductor nanoparticles and offer insights into precisely tuning the band gap energy and tailoring optical properties to optimize electronic performance for specific applications.

Presenter: Ho Khac Hieu

P.26 – Poster, VCTP-50

Half-metal state in honeycomb lattice with defects

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A theoretical model for graphene-like structures with regular atom doping is studied. The model is based on the Hubbard model on a honeycomb lattice with regular defects. An iterative perturbation approximation is employed to investigate both the electronic and magnetic structures. It is found that a half-metal state may be realized when electrons at the defect sites can hop to surrounding sites and the bare energy levels of two honeycomb sublattices are different. When the defects are isolated, the ground state is ferrimagnetic and opens an energy gap. A possibility of relating to graphitic carbon nitride materials is also discussed.

Presenter: Nguyen Hong-Son

P.27 – Poster, VCTP-50

This computational research delves into the electronic, magnetic, and spin transport phenomena observed in rich spin penta-PdSe2 nanoribbons

Nguyen Hai Dang (1,2), Pham Thi Bich Thao (1), Nguyen Duy Khanh (3) and Nguyen Thanh Tien (1)

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Using spin-polarized DFT calculations combined with the non-equilibrium Green's function (NEGF) method, we investigated the geometric, electronic, magnetic, and spin transport properties of bare-edge and H-edge ZZ-p-PdSe2 nanoribbons across six distinct spin configurations. Our findings reveal the robust stability of these nanoribbons, a direct-gap semiconducting nature with varying spin-splitting bandgaps, and diverse magnetic behaviors ranging from ferromagnetic to antiferromagnetic depending on the spin configuration. Critically, the spin-resolved I-V curves highlight prominent negative differential resistance (NDR) and spin filtering (SF) effects, with detailed mechanisms elucidated through transmission spectra, carrier paths, and local density of states. These results provide a comprehensive understanding of penta-PdSe2 nanoribbons, offering valuable insights for the development of spintronic devices leveraging this emergent system.

Presenter: Nguyen Hai Dang

P.28 – Poster, VCTP-50

The Debye-Callaway model for thermal conductivity calculation of black phosphorus nanoribbons

Nguyen Viet Chien

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Thermal conductivity (κ) in solids consists of contributions from both electronic thermal conductivity (κ_e) and lattice thermal conductivity (κ_l), with the latter often significantly reduced in low-dimensional materials. Understanding phonon transport in these systems requires reliable modeling of κ_l. The Debye-Callaway model, derived from the phonon Boltzmann transport equation, provides a robust theoretical framework by incorporating key phonon scattering mechanisms. In this study, we apply the Debye-Callaway model to analyze the lattice thermal conductivity of black phosphorus (BP) nanoribbons synthesized via chemical vapor transport (CVT) at different growth rates (7, 0.3, and 0.05 K/min). Experimental κ_l data, obtained using a suspended microdevice, show a significant increase in the 50–200 K range as the growth rate

decreases, suggesting enhanced phonon transport. Fitting the experimental data to the Debye-Callaway model, while accounting for boundary, point defect, Normal, and Umklapp scattering, indicates that this enhancement arises primarily from the suppression of phonon–point defect scattering, consistent with improved crystalline quality at lower growth rates. Our results confirm the Debye-Callaway model's effectiveness in linking phonon scattering to microstructural quality, providing key insights into thermal transport in BP nanoribbons and related nanomaterials.

Presenter: Nguyen Viet Chien

P.29 – Poster, VCTP-50

Design and Optimization of Multilayer Metamaterial Perfect Absorbers for Broadband Solar Energy Harvesting

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Multilayer metamaterial-based broadband absorbers have emerged as promising candidates for advanced solar energy harvesting due to their ability to achieve near-perfect absorption across a broad spectral range (0.3–2.5 μm), which covers the majority of the solar spectrum. Their flat form is the simplest structure and make them fabricated easily. In this study, we design and optimize three different multilayer metamaterial perfect absorbers for solar energy applications. One of our metamaterials has the averaged absorption across the spectral wavelength higher than 93

Presenter: Do Thi Nga

P.30 – Poster, VCTP-50

Collective excited states at small amplitude in neutron elastic scattering at low-energies

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We investigate the contributions of isoscalar and isovector collective excitations in the neutron elastic scattering of 16O, 40Ca, 48Ca, and 208Pb nuclei by using a microscopic optical potential (MOP) derived from nuclear structure models based on self-consistent mean-field approaches. Particular attention is given to the role of these collective modes in shaping the imaginary part of the MOP and the resulting angular distributions. Our analysis indicates that both isoscalar and isovector contributions are significant for all considered targets, especially for light and medium targets. Furthermore, the Coulomb interaction is found to play an important role in describing absorption mechanisms and reproducing the experimental angular distributions [1].

[1] submitted to Physical Review C (2025).

Presenter: Do Quang Tam

P.31 – Poster, VCTP-50

First-Principles Study of Hydrogen Cyanide Captured on M2CO2 (M = Sc, Ti, V) MXenes

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Hydrogen cyanide (HCN) is highly poisonous to the human nervous system, even with a small dose. The detection of HCN has been extensively studied using various types of typical adsorbents, including both metal oxides and functionalized carbonaceous materials. MXenes, a family of two-dimensional materials, propose new media for HCN adsorption and recognition. This work reports the capture and sensing performance of M2C and M2CO2 MXenes (M = Sc, Ti, V) toward HCN studied by first-principles density functional theory calculations (DFT). Insight analysis of the charge density difference, electron localization function, density of state, and band structure allows us to determine the bonding mechanisms and electronic structure changes upon the adsorption of HCN on the studied surfaces. The detection performance is evaluated through the recovery time and sensitivity. HCN molecules are stable at their most favorable adsorption sites at room temperature, revealed by ab initio molecular dynamics simulations (AIMD).

Presenter: Le Nguyen-Minh Thong

P.32 – Poster, VCTP-50

Qutrit-based simulation of collective three-flavor neutrino oscillations

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In this work, we present a quantum simulation approach to model the collective behavior of three-flavor neutrinos using qutrit-based quantum circuits. Each neutrino is represented by a

qutrit—a quantum system with three energy levels—allowing a natural encoding of the SU(3) flavor structure. We use the Trotter–Suzuki decomposition to approximate the time evolution generated by the collective Hamiltonian. We then design quantum circuits composed of qutrit gates corresponding to these decomposed unitary operators. The simulation results show that the qutrit framework can effectively reproduce key features of three-flavor oscillations.

Presenter: Vũ Văn Hướng

P.33 – Poster, VCTP-50

The Dimerization of the Aβ42 under the Influence of the Gold Nanoparticle: A REMD Study

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ABSTRACT: Advances in Alzheimer's disease (AD) are related to the oligomerization of Amyloid beta (Aβ) peptides. Therefore, alteration of the process can prevent AD. We investigated the Aβ42 dimerization under effects of gold nanoparticles using temperature replica-exchange molecular dynamics (REMD) simulations. The structural change of dimers in the presence and absence of the gold nanoparticle, Au55, was monitored over the stable intervals. Physical insights into the oligomerization of the Aβ were thus clarified. The computed metrics indicate that Au55 affects the progress of oligomerization. Specifically, the presence of the gold nanoparticle significantly modifies the structure of the dimeric Aβ42. The β-content experienced a substantial decrease with the induction of Au55. The turn- and coil-contents are also decreased under the effects of the gold nanoparticle. However, the α-content of the dimer exhibited a rigid increase. The influence of gold nanoparticle on the dimeric Aβ42 differs significantly from that of silver nanoparticles, which reduce β-content but increase coil-, turn-, and α-contents. The nature of inhibition would be discussed, in which the vdW interaction plays a driving force for the interaction between the Aβ42 dimer and the gold nanoparticle.

Presenter: Ngo Son Tung

P.34 – Poster, VCTP-50

Optical transitions and Hofstadter spectra of monolayer TMDCs: a tight-binding investigation

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(2) Institute of Advanced technology, Vietnam Academy of Science and technology

We investigate optical transitions and Hofstadter spectra of group-VIB transition metal dichalco-

genide monolayers using a three-band tight-binding model with up to third-nearest-neighbor hoppings. For zero magnetic field, we calculate the optical matrix elements as well as the optical selection rules and compare them with the results from the k.p and ab-initio methods. In the presence of an external magnetic field, the calculated band energies show Landau levels at small fields and become fractal-structured at strong fields, which is known as the Hofstadter butterfly.

Presenter: Tran Khoi Nguyen

P.35 – Poster, VCTP-50

Regulated perturbation theory for anisotropic 2d exciton and a variable separation procedure for complicated double integrals

Le Do Dang Khoa, Le Hoang Viet, Le Van Hoang

Ho Chi Minh City University of Education

After the success of graphene, a series of new two-dimensional materials were born with many important applications in optoelectronics. Exciton plays an important role in the research and development of two-dimensional semiconductor materials and has been widely studied over the years. In this paper, we develop and improving the regulated perturbation theory for anisotropic exciton base on an algebraic method approach to the calculation of energy spectrum and wavefunction of exciton in black phosphorus monolayer which has an anisotropic structure. The regulated perturbation theory is the theory of combining the perturbation method and Feranchuk-Komarov operator method. These methods include the scaling space, Levi-Civita transformation, the algebraic calculation using the annihilation and creation operators, and introduction to the free parameter which have a role in optimize the convergence rate. At the same time, a computational procedure is proposed for evaluating a specific form of double integral that characterizes the anisotropic structure of black phosphorus (BP). This integral exhibits a highly complicated form, and the proposed method significantly reduces the computational cost—by up to hundreds of thousands of times. Our results are highly accurate up to six decimal places for both energy spectrum and wavefunction and well agreement with the experiment. These results are an important step, promoting research on excitons in anisotropic monolayers by algebraic and analytical methods later.

Presenter: Le Do Dang Khoa

P.36 – Poster, VCTP-50

Dynamical Optical Absorption of a Monolayer Graphene inside an Empty Optical Microcavities

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The optical absorption on the graphene monolayer is usually examined using the static conductivity [1, 2]. In this study, using the dynamical conductivity, we examine in detail the absorption of the graphene layer inserted inside in empty optical microcavity. The optical conductivity of monolayer graphene is modeled using the Kubo formalism. Our results show that the optical force can increase several tens of time of magnitude in comparison to that in the case without the cavity. Especially, the optical absorption could be effectively tuned by varying the graphene's position within the cavity and the cavity length, i.e. the distance between the two reflective mirrors. These findings not only advance the understanding of light–matter interaction in hybrid photonic systems but also optimize the design and performance of graphene-based optical devices.

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Presenter: Pham Nguyen Thanh Vinh

P.37 – Poster, VCTP-50

Two-component dark matter from a flavor-dependent U(1) extension of the standard model

Duong Van Loi, Nguyen Hoang Duy, N. T. Duy

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We present a flavor-dependent $U(1)_X$ gauge extension of the standard model that naturally explains the number of fermion families, generates small neutrino masses via the scotogenic mechanism, and predicts two stable dark matter candidates. This leads to a two-component dark matter scenario with rich phenomenology. The model also features flavor-dependent couplings and a new gauge boson Z', offering testable signatures via flavor-changing neutral currents and collider searches.

Presenter: Duong Van Loi

P.38 – Poster, VCTP-50

Effect of temperature and pressure on thermodynamic and melting properties of HP2 structure thallium metal

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In this work, we apply the Debye model to study the effects of temperature and pressure on some thermodynamic quantities of HP2-structured Thallium metal, in which the analytical expressions of the anharmonic effective potential, the effective force constant, the Debye frequency, the Debye temperature and the Debye-Waller factor are derived as functions of the axis ratio e = c/a and pressure. The pressure-dependent melting properties of Thallium are also studied by us based on the Lindemann melting model. The previously relevant experimental parameters are used by us to numerically calculate of these thermodynamic quantities up to a temperature of 700 K and a pressure of 50 GPa. Our findings indicate that the anharmonicity of the thermal lattice

vibrations and pressure significantly affects the thermodynamic quantities of Thallium metal. Our calculated melting curve of Thallium agrees well with the theoretical and experimental results reported in previous studies. This study not only expands the understanding of the thermodynamic properties and melting behavior of Thallium metal, but can also be used to predict and calculate the thermodynamic properties, melting behavior of other metals and alloys in harsh environments

Presenter: Nguyen Thi Hong

P.39 – Poster, VCTP-50

Neutrinoless double beta decay in an extended model with left-right symmetry

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In this report, we examine the phenomenology of the neutrinoless double beta decay in the framework of a left-right symmetric model based on extended gauge symmetry $SU(3)_C \otimes SU(3)_L \otimes SU(3)_R \otimes U(1)_X$. We will mainly concentrate on the contributions of new physics on the neutrinoless double beta decay effective mass and its sensitivities to the shortcoming experiments.

Presenter: Dinh Nguyen Dinh

P.40 – Poster, VCTP-50

Controlling displacement of warp drive spaceship system using Proportional –Integral–Derivative controller

Tran Dinh An

HCMC university of Technology and Education

In 1994, Miguel Alcubierre proposed the warp drive engine model, in which a spaceship equipped with such an engine could travel through space by curving spacetime, allowing it to move faster than the speed of light. In this research, I focus on solving the control problem of displacement along a single spatial axis of a spaceship equipped with a warp drive engine, modeled in the Cartesian coordinate system. The analysis is based on the nonlinear differential equation (12) presented in Alcubierre's original paper [1].By employing an approximate linearization method combined with Taylor series expansion, followed by the Laplace transform to derive the transfer function between spacetime curvature and spatial displacement, incorporating assumed mathematical transfer functions for the subsystem components, a generalized transfer function of the entire warp-drive spaceship system is obtained. From this, control theory is applied to design a PID controller, which is a controller that regulates the system based on the error between the reference input and the output variable over time. The PID parameter tuning methods is used for controller design, and mathematical criteria are employed to analyze the stability of the closed-loop system.

Presenter: Trần Đình An

P.41 – Poster, VCTP-50

Electronic and thermoelectric properties of WO3 under the adsorption of volatile organic compounds: first-principle study

Phan Thi Hong Hoa (1,2), Do Ngoc Son (1,2)

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Cancers release certain volatile organic compounds in the patient's breath. Early-stage and non-invasive diagnosis via sensors has attracted much attention from researchers. WO3 is a candidate for sensor materials, whereas no study has been published to clarify the electronic and thermoelectric properties of this material for detecting volatile organic compounds. By the density functional theory calculations, we clarified the properties of WO3 upon the adsorption of volatile organic compounds.

Presenter: Phan Thi Hong Hoa

P.42 – Poster, VCTP-50

Light absorbed by Dirac electrons in silicene under a non-uniform magnetic field

Huynh V. Phuc (1), Pham T. Vinh (1), Bui N. Thu (1), Tran N. Bich (2), Le T. Hoa (3), Le Dinh (3)

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(2) The University of Da Nang;
(3) Hue University

We study the magneto-optical absorption of Dirac electrons in monolayer silicene under a perpendicular electric field and a non-uniform magnetic field. Using the equation of motion method within linear response theory, we compute longitudinal and Hall susceptibilities, focusing on both intraband and interband transitions. The optical response is strongly dependent on electron density, which shifts the Fermi level and modifies transition pathways. Higher densities lead to blue-shifted interband thresholds and enhanced intraband peaks. Circular polarization plays a key role: left-handed light enhances absorption, while right-handed light suppresses it. A characteristic "half-peak" emerges due to asymmetric Pauli blocking. While the magnetic field effectively tunes the absorption spectrum through Landau level modulation, the electric field has a weaker influence under strong quantization. These results highlight the tunable magneto-optical behavior of Dirac electrons in silicene, suggesting potential applications in polarization-sensitive and field-controlled optoelectronic devices.

Presenter: Huynh V. Phuc

P.43 – Poster, VCTP-50

The Hall Effect in an infinite Semi-parabolic Plus Semi-inverse Squared Quantum wells in the presence of a Strong Electromagnetic Wave.

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The Hall Effects (HE) in an infinite Semi-parabolic Plus Semi-inverse Squared Quantum wells (ISPPSISQW) in the presence of a strong Electromagnetic Wave (EMW) is theoretically investigated by using Quantum Kinetic Equation. The system is subjected to a strong EMW $E(t) = (E_0 \sin \Omega t)e_y$, a magnetic field $B = Be_z$, and a cross-DC electric field $E = Ee_x$. The

electron-optical phonon scattering is considered. The general expression of the Hall coefficient is presented as a function of the temperature, the external magnetic field, the photon energy, and the intensity of the strong EMW as well as characteristic parameters of ISPPSISQW. The theoretical result for a specific GaAs/GaAsAl ISPPSISQW is achieved by using the numerical method. The computational results demonstrate that the maximum peaks appear to satisfy the magneto-phonon-photon resonance condition. Regarding the dependence of the Hall Coefficient on the magnetic field B: when the temperature changes, the position of the resonance peak remains unaffected by temperature variations; and when the confinement frequency increases, the magnitude of the Hall coefficient peak increases, and the position of the peak shifts towards the smaller magnetic field B. For the dependence of the Hall Coefficient on the electromagnetic wave frequency: when the temperature changes, the peak decreases, but the position of the peak does not change; and when increasing confinement frequency, the magnitude of the peak increases; and when the external magnetic field B increases, the magnitude of the Hall coefficient increases and the peak position shifts towards the higher frequencies.

Presenter: Bui Thi Dung

P.44 – Poster, VCTP-50

`Darksuite`: an Algorithm for Dark-Matter Admixed Neutron Stars

Nguyen Thi Lan Anh (1), Peter Lott (1), Nguyen Quynh Lan (1)

(1) Phenikaa University

Gravitational-wave observations provide a unique window into the fundamental nature of massive objects. In particular, neutron star equations of state have been constrained due to the success of gravitational wave observatories. Recently, the possibility of detecting dark matter admixed neutron stars via ground-based laser interferometry has been explored. Dark matter would impact the gravitational waveform of an inspiraling neutron star system through tidal parameters, namely the tidal deformability (λ), incurring a phase shift to the frequency evolution of the signal. The phase shift depends both on the percentage of dark matter within the star and its particle nature, e.g. bosonic or fermionic. If detected, indirect detection of dark matter through admixture within neutron stars can provide insight into the neutron equation of state, as well as constraints on the density of dark matter in the universe. In this paper, we introduce `Darksuite`, a proposed extension of `LALSuite` aimed at incorporating light dark matter effects into gravitational waveform models. This framework employs simulations from the two-fluid, generally relativistic Tolman-Oppenheimer-Volkoff equations, wherein one fluid is ordinary nuclear matter and the other is dark matter. We demonstrate interpolation of values from a bank of simulations, enabling the study of binary systems where at least one component may be a dark-matter-admixed neutron star. By leveraging existing methodologies within `LALSuite` for tidal phase corrections and supplementing them with dark matter effects, `Darksuite` provides a means to generate and analyze gravitational waveforms for these exotic systems. In the future, we hope to systematically assess the influence of dark matter on waveform morphology, explore the detectability of these effects with current and next-generation observatories, and refine constraints on dark matter properties through gravitational wave observations.

Presenter: Nguyen Thi Lan Anh

P.45 – Poster, VCTP-50

Modeling Myopia Progression through an Evolution Equation: Interactions Between Stimulus, Attention, and Eye Elasticity

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Abstract. The rapid rise in myopia prevalence globally underscores the need for a mechanistic understanding of eye growth regulation. While genetic predisposition contributes, recent evidence strongly implicates visual behavior and environmental factors, especially near work and outdoor light exposure—as critical drivers of refractive development. This study proposes a novel Eye Evolution Model (EEM) describing myopia progression as a dynamic interplay between optical stimuli, behavioral patterns, and age-dependent ocular biomechanical properties. Inspired by viscoelastic and RC-charging analogies, the EEM describes axial elongation as a stimulus-response process regulated by a mechanical time constant (τ), reflecting ocular elasticity and compliance. The model introduces a lifestyle modulation term to account for cumulative visual tasks influenced by behavioral continuity and intensity. Unlike previous empirical models, this mechanistic approach explains observed phenomena such as stabilization of moderate myopia, accelerated progression following full correction, and refractive stability during inattentive vision or sleep. Unlike probabilistic models, the EEM reveals that refractive change emerges only when environmental, behavioral, and biological factors interact simultaneously highlighting their multiplicative, not additive, relationship. The EEM offers new insights into longstanding debates regarding defocus, accommodation, and behavioral influences on myopia. By quantifying environmental, behavioral, and biomechanical contributions, the EEM provides a foundation for personalized strategies to predict and control myopia progression.

Keywords: myopia progression, emmetropia, axial elongation, evolution model, evolution equation

Presenter: Nguyễn Văn Hoa

P.46 – Poster, VCTP-50

Interface Engineering and Electric Contact Design of two-dimensional van der Waals Heterostructure for Flexible Electronics

Pham T. Truong (1,2), Le M. Duc (3), Nguyen V. Hieu (4), Nguyen N. Hieu (5), Huynh V. Phuc (2), Tran P. T. Linh (6), Nguyen T. Hiep (5), Nguyen Q. Cuong (5), Vo T. T. Vi (7), Nguyen Văn Chuong (3)*

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(7) Hue University of Medicine and Pharmacy

In this work, we employ density functional theory (DFT)-based first-principles calculations to

design and investigate a series of two-dimensional (2D) metal-semiconductor (MS) heterostructures, systematically exploring their electronic structures and interfacial properties. The contact behaviors, including Schottky-to-Ohmic transitions, are comprehensively analyzed, with particular emphasis on the tunability of Schottky barrier heights via interface engineering. Furthermore, we demonstrate potential strategies for reversible control over contact characteristics through external perturbations, offering avenues for adaptive electronic functionalities. The insights gained from this study not only deepen the understanding of interfacial phenomena in 2D heterostructures but also provide a theoretical foundation for the rational design of low-resistance, high-performance contacts in next-generation nanoelectronic devices.

Presenter: Nguyễn Văn Chương

P.47 – Poster, VCTP-50 **Elucidating H_2S adsorption on activated carbon by van der Waals corrected density functional theory calculations**

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Effective removal of hydrogen sulfide (H_2S) from biogas is essential not only for environmental protection and human health but also for enabling the safe utilization of biogas, for example in domestic cooking. This is particularly important in the context of Vietnamese agriculture, where biogas is widely used as a renewable energy source in rural areas. Among various removal techniques, H_2S capture from biogas via the adsorption process using activated carbon (AC) adsorbent is particularly attractive due to its high efficiency, low energy consumption, and operational simpliCity. A fundamental understanding of the H_2S adsorption mechanism at the atomic level is critical for optimizing AC adsorbent. In this work, we investigate the adsorption behavior of H_2S on AC using van der Waals (vdW) Density Functional Theory (DFT) calculations. AC was modeled by coronene and graphene structures and all possible H_2S adsorption sites on both coronene and graphene were explored. The results indicate that van der Waals interactions dominate the adsorption of H_2S on both coronene and graphene surfaces. Further electronic structure analysis including the projected density of states (PDOS), and Löwdin population reveals the interaction mechanisms between H_2S and AC surfaces. The results provide insights for designing efficient materials for gas purification and environmental applications. The details of our work will be presented at the conference.

Presenter: Nguyen Le Bao Tran

P.48 – Poster, VCTP-50

Retrieving Anharmonic Interatomic Potentials from Conventional and Laser-Induced Electron Diffraction

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Retrieving structural information and interatomic potentials from electron diffraction is essen-

tial for understanding molecular dynamics at the quantum level. While conventional electron diffraction (CED) has long been used for static imaging, laser-induced electron diffraction (LIED) offers femtosecond-scale temporal resolution, enabling real-time tracking of structural changes. However, the role of nuclear vibrations in shaping diffraction signals remains underexplored, especially in LIED where intense laser fields can amplify vibrational effects. The goal of this study is to assess the influence of nuclear vibrations on diffraction patterns and to evaluate whether anharmonic interatomic potentials can be reconstructed from both CED and LIED signals. We simulate diffraction images for both methods, incorporating thermal nuclear motion in CED and laser-induced vibrations in LIED. In the CED case, we find that diffraction images are most sensitive to interatomic distance, while sensitivity to anharmonic Morse parameters is weaker but still measurable with high precision. In LIED, we develop a method to include laser-driven nuclear dynamics and show that intense laser fields broaden the nuclear wavepacket, enhance population of higher vibrational levels, and significantly increase sensitivity to anharmonic potential shapes. These results demonstrate that LIED is a viable route for reconstructing anharmonic interatomic potentials, with broader applicability beyond the Morse model used in this work.

Presenter: Nguyễn Thị Hiền

P.49 – Poster, VCTP-50

Impact of nuclear reaction cross sections on primordial deuterium abundance

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Radiative capture reactions critically determine primordial deuterium production during Big Bang nucleosynthesis (BBN). A microscopic potential model is employed to calculate electromagnetic transition matrix elements and updated astrophysical S-factors. The corresponding reaction rates are implemented in a 40-reaction BBN network, yielding a deuterium-to-hydrogen ratio in excellent agreement with Lyman-alpha absorption measurements of high-redshift gas clouds. The study highlights the strong sensitivity of BBN predictions to low-energy nuclear inputs and provides tighter constraints on the cosmic baryon density.

Presenter: Dao Nhut Anh

P.50 – Poster, VCTP-50

Emergent Localized Electronic States and Phonon Suppression in V_2WO_6 : A New Class of Oxide Thermoelectric Materials

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We present a comprehensive theoretical and experimental investigation of V_2WO_6, an oxide that couples Anderson-like electronic localization with strong phonon scattering to enable promising thermoelectric performance. Density-functional theory and transport measurements show that electronic conduction is strongly influenced by localized states near the Fermi level, consistent

with Anderson localization and Mott-type correlations within vanadium d-orbitals. This coexistence of itinerant and localized carriers preserves a large Seebeck coefficient ($\sim -395\ \mu\mathrm{V,K}^{-1}$ at 300 K). Phonon-dispersion spectra reveal softened acoustic modes and extensive acoustic–optical coupling, driving intrinsic phonon-glass behavior. Consequently, the total thermal conductivity remains as low as $\sim 0.9\ \mathrm{W,m}^{-1},\mathrm{K}^{-1}$ over a wide temperature range, falling to a lattice component of $\sim 0.18\ \mathrm{W,m}^{-1},\mathrm{K}^{-1}$ at high temperatures. These coupled electronic and phononic features yield a peak thermoelectric figure of merit $zT \approx 0.42$ at 900 K in pristine polycrystalline samples. V_2WO_6 thus emerges as a prototype for designing oxide thermoelectrics that harness correlated electronic localization alongside engineered phonon suppression, offering a fresh pathway toward high-performance, thermally robust energy-conversion materials.

Presenter: Le Nguyen Ngoc Quy

P.51 – Poster, VCTP-50

$(g-2)_{e,\mu}$ and lepton flavor violating decays in a left-right model

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General expressions for one-loop contributions associated with lepton-flavor violating decays of the standard model-like Higgs boson $h \to e_b^{\pm} e_a^{\mp}$ and gauge boson $Z \to e_b^{\pm} e_a^{\mp}$ are introduced in the unitary gauge. The results are used to discuss these decays as new physics signals in a minimal left-right symmetric model containing only one bidoublet Higgs and a $SU(2)_R$ Higgs doublet accommodating data of neutrino oscillations and $(g-2)_{\mu}$. The numerical investigation indicates that some of these decay rates can reach near future experimental sensitivities.

Presenter: Nguyen Hua Thanh Nha

P.52 – Poster, VCTP-50

Orientation asymmetry of planar molecules reflected in high-harmonic generation spectra

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High-order harmonic generation (HHG) has emerged as a powerful tool for probing molecular electronic structure [1,2] and dynamics [2,3]. Numerous studies have shown that the HHG spectra emitted from linear polar molecules can exhibit both odd and even harmonics when the symmetry of the laser – target system is broken, typically due to the intrinsic permanent dipole moment of the molecule. Recent research further reveals that the intensity ratio between even and odd harmonic orders – referred to as even-to-odd ratio [4], and the phase difference between two consecutive HHG bursts contributing to the same harmonic order [5], remain stable under different laser conditions and can be used to characterize the molecule's intrinsic asymmetry [4,5]. However, these research have so far focused on linear polar molecules. For nonlinear molecules with symmetric geometric structures, there still exist certain orientations for which the two-fold rotational symmetry is broken. The use of HHG spectra to characterize the directional asymmetry of such molecules has not yet been systematically investigated. In this study, we employ time-dependent density functional theory (TDDFT) to simulate HHG from the planar, C_3-symmetric molecule BH_3. We analyze two key observables extracted from the HHG signal: the even-to-odd ratio and the phase difference between two consecutive HHG bursts, as functions of the laser polarization direction. Our results show that the HHG spectra vary significantly with the polarization direction, transitioning from purely odd harmonics to mixed odd-even harmonics and then back to purely odd. This behavior directly reflects the directional asymmetry in the molecular structure. Notably, this phenomenon is observed not only for the highest occupied molecular orbital (HOMO) but also persists for lower-lying orbitals such as HOMO-1. Furthermore, when using few-cycle laser pulses with suitable wavelengths, the extracted even-to-odd ratio and phase difference can even reconstruct the geometric and electronic asymmetry of the molecule along different orientations.

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Presenter: Trần Thành

P.53 – Poster, VCTP-50

Studying nonclassical properties of the superposition of photon-added and photon-subtracted single-mode displaced Fock state

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In this study, the superposition of photon-added and -subtracted single-mode displaced Fock state (S-PAS-SMDFS) is a class of nonclassical states that we construct by applying a super-

position technique of photon addition and subtraction to the single-mode displaced Fock state (SMDFS). This technique significantly modifies the properties of the original SMDFS, resulting in a strongly non-Gaussian state characterised by the negativity of its Wigner function. Our study demonstrates that the S-PAS-SMDFS exhibits prominent nonclassical features such as higher-order squeezing properties in the type of Hillery and antibunching properties. Notably, these nonclassical characteristics are more pronounced than those observed in states generated by solely adding, subtracting, or simultaneously adding and subtracting photons without using the superposition technique. These findings highlight the effectiveness of the superposition technique in enhancing the nonclassical properties of quantum states.

Presenter: Ho Sy Chuong

P.54 – Poster, VCTP-50

Investigation of thermodynamic properties of ideal classical and quantum gases in one-, two-, and three-dimensional space.

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The thermodynamic functions of classical and quantum ideal gases have been extensively investigated using analytical and numerical methods, playing a significant role in statistical physics. The examination of these thermodynamic functions is of particular significance to students, as it is a fundamental stage in the comprehension of physical systems at low temperatures and quantum effects. This work involves the explicit temperature dependence of thermodynamic functions, including total energy, heat capacity at constant volume, entropy, and Gibbs free energy, for classical and quantum ideal gases in one-, two-, and three-dimensional spaces. Analytical calculations are conducted. The statistical properties of the Maxwell-Boltzmann, Fermi-Dirac, and Bose-Einstein distribution functions are combined with the grand canonical ensemble to underpin the approach. The validity range of the derived formulas is determined by comparing the analytical expressions with numerical results, which assesses their applicability and accuracy.

Presenter: Phan Quang Sơn

P.55 – Poster, VCTP-50

A renormalizable neutrino mass model with $(Z_2 \times Z_4) \rtimes Z_2$ (II) symmetry

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A renormalizable neutrino mass model based on $(Z_2 \times Z_4) \rtimes Z_2$ (II) symmetry is proposed for the modification of the $\mu - \tau$ reflection symmetry. The hierarchies of lepton masses can be naturally realized and the lepton mixing is addressed with renormalizable Yukawa couplings. The predicted intervals of the sum of neutrino mass and the Majorana effective neutrino mass are consistent with the corresponding experimental limits.

Presenter: Trần Đình Thám

P.56 – Poster, VCTP-50

The effect of oxygen vacancy concentration on structural, electronic and optical properties of Bi_2WO_6 photocatalyst: DFT study

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In this study, the effects of oxygen vacancy (OV) concentration on the structural, electronic, and optical properties of Bi_2WO_6 photocatalyst were systematically investigated using density functional theory (DFT). Six different oxygen-deficient models were constructed with vacancy concentrations ranging from 0 to 25%, corresponding to 1–6 missing oxygen atoms in the Bi_2WO_6 lattice. Structural analysis revealed that increasing OV concentration induces significant lattice distortion, modifies Bi-O coordination environments, and affects unit cell parameters, especially causing abrupt expansion along the b-axis and unit cell volume at higher defect densities. Electronic structure calculations show that the introduction of OVs creates impurity states near the conduction band, resulting in reduced band gap energy from 2.326 eV to below 0.5 eV. Electron density difference (EDD) maps and Bader charge analysis indicate progressive electron accumulation near vacancy sites, suggesting the formation of F-centers and partial reduction of Bi^{3+} to Bi^{2+}. These electronic modifications enhance the n-type conductivity of Bi_2WO_6. Optical property analysis demonstrates a visible-light red-shift in absorption edges and the emergence of new low-energy peaks in both absorption and dielectric function spectra, attributed to OV-induced defect states. The results suggest that moderate oxygen vacancy concentrations can effectively tune the electronic structure and optical response of Bi_2WO_6, offering a promising strategy to enhance its photocatalytic performance.

Presenter: Doan Thi Hien

P.57 – Poster, VCTP-50

Modeling Gravitational Wave Signatures from Magnetars Using Generally-Relativistic Magnetohydrodynamic Simulations

Nguyen Thi Thao Trang (1), Lott Peter Tell (1), Nguyen Quynh Lan (1)

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Magnetars, highly magnetized neutron stars, generate gravitational waves through asymmetries in their crust and magnetic field, often referred to as "mountains". These deformations arise from strong magnetic stresses and rotational forces, leading to a time-varying mass quadrupole moment that produces gravitational wave emission within the detectability band of current

ground-based detectors. We employ Athena++, a general relativistic magnetohydrodynamic framework, to simulate a physically realistic magnetar, initializing a strong dipolar magnetic field and introducing a localized deformation in the crust. The simulation evolves under fully relativistic conditions, capturing the coupled effects of magnetic stress, rotational forces, and hydrodynamic feedback. We extract gravitational waveforms using the quadrupole approximation and analyze through Fourier transforms to uncover dominant frequency components and their temporal evolution. A parameter study across magnetic field strengths, deformation scales, and rotation rates reveals the optimal conditions for generating detectable gravitational wave signals. When compared against the sensitivity curves of ground-based gravitational-wave detectors, the results suggest that certain magnetar configurations may produce marginally detectable signals. This work may be relevant for search for long-term signals from mountains on magnetars.

Presenter: Nguyen Thi Thao Trang

P.58 – Poster, VCTP-50

Solving bound and scattering problems using symmetric matrix techniques

Nguyen Gia Huy

Ho Chi Minh City University of Education (HCMUE)

This study presents a numerical method for solving the matrix Schrödinger equation using symmetric tridiagonal and heptadiagonal matrices. It is applied to compute bound and scattering states in the cases: a one-body problem with a square well potential using natural units; the nuclear structure and scattering of the $n+^{16}$O system with physical parameters; and the deuteron structure using the Malfliet–Tjon potential. The numerical results are compared with analytical solutions and alternative computational methods. These comparisons demonstrate that the symmetric heptadiagonal matrix offers improved accuracy, particularly in calculating phase shifts for scattering states.

Presenter: Nguyen Gia Huy

P.59 – Poster, VCTP-50

Reflection coefficient of a superconducting artificial atom coupled to a mirror

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Qubit readout plays a crucial role in quantum research, as it enables the extraction of fundamental properties such as the qubit's operating frequency and coherence time through the analysis of reflected and transmitted signals. In the case of superconducting qubits, we consider the Cooper Pair Box model, which functions as an artificial atom coupled to a transmission line—one end of which is open to infinity, while the other is connected to a capacitor that acts as a mirror, reflecting electromagnetic waves. To determine the reflection coefficient of this system, we employ methods from circuit quantum electrodynamics, transmission line theory, and theory of open quantum systems, combined with plotting the reflection coefficient using Python. The analysis is conducted in two regimes: when the artificial atom behaves as a harmonic oscillator and when it exhibits true qubit-like behavior. This allows us to investigate how the position of the artificial atom affects the reflection spectrum.

Presenter: Tran Thi Thanh Huyen

P.60 – Poster, VCTP-50

Evaluation of nuclear level density dependence on quadrupole deformation in ^{56}Fe nuclei

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The nuclear level density (NLD) of ^{56}Fe was studied using the exact pairing plus independent particle model (EP + IPM) [1], and the results were compared with experimental data for a range of quadrupole deformation parameters, either assumed or obtained from theoretical and experimental sources [2, 3]. The results indicate that quadrupole deformation, represented by the parameter β_2, significantly influences the NLD, particularly at low excitation energies. This influence is primarily attributed to changes in the nuclear potential shape, which affect the distribution and density of energy levels.

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Presenter: Le Thi Quynh Huong

P.61 – Poster, VCTP-50

Thermoelectric properties in tilted 8-Pmmn borophene

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We study the thermoelectric transport properties of gapped tilted-8-Pmmn borophene—a two-dimensional boron allotrope characterized by anisotropic electronic dispersion—using semiclassical Boltzmann transport theory under the constant relaxation time approximation. The low-energy effective Hamiltonian includes a tilted Dirac cone structure with a strain- or substrate-induced bandgap. We compute the electrical conductivity, Seebeck coefficient, and thermopower as functions of chemical potential, energy gap, and temperature. Our analysis reveals strong anisotropy in transport behavior between the x- and y-directions, with the x-direction showing superior conductivity and thermopower. Increasing the bandgap enhances the Seebeck coefficient and thermopower by bringing the Fermi level closer to the band edges, whereas higher temperatures improve electrical conductivity but reduce the Seebeck coefficient. These results underscore the promise of gapped 8-Pmmn borophene for nanoscale thermoelectric device applications.

Presenter: Bui Dinh Hoi

P.62 – Poster, VCTP-50

Optically controlled spin transport in topological insulator thin films

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We explore the spin Edelstein effect at low temperatures in topological insulator thin films irradiated with circularly polarized light. Employing a high-frequency Floquet framework, we derive an effective Hamiltonian that captures the light-induced modifications to the mass gap and Fermi veloCity. Using this model, we calculate the spin Edelstein susceptibility via Kubo linear response theory, incorporating both intraband and interband contributions. Our results reveal that optical driving enables significant tunability of spin polarization, with critical behavior emerging near a Floquet-engineered topological phase transition, where the effective Fermi velocity approaches zero. We further show that surface asymmetry, hybridization strength, and interband relaxation processes critically influence the spin response. These findings highlight the potential for dynamic optical control of spin accumulation in topological materials, opening new avenues for spintronic device applications.

Presenter: Le Thi Thu Phuong

P.63 – Poster, VCTP-50

Molecular mechanism of Ensitrelvir and its similarity inhibiting SARS-CoV-2 main protease by molecular dynamics simulation

Huynh Thi Ngoc Thanh (1), Kieu Minh Nhan (1), Kieu Nhat Ha (1), Nguyen Quoc Thai (1)

(1) Dong Thap University

The unprecedented challenge posed by the COVID-19 pandemic, driven by SARS-CoV-2, has emerged as a global threat. In response, a limited array of therapeutics has been approved for the prevention and treatment of SARS-CoV-2 infection. The main protease (Mpro) of SARS-CoV-2 has been a significant target for drug development efforts because of its crucial role in the viral replication process. This study is to investigate the efficacy of Ensitrelvir and its derivatives in inhibiting the mechanism of the Mpro target of SAR-CoV-2. Docking simulation and molecular dynamic simulation (SMD) techniques were employed for this purpose. The results indicate that the CID 166498740 derivative obtained affinity energy-9.3 kcal/mol and rupture force (Fmax) 638.3 ± 79.3 (pN), which proved that the CID 166498740 derivative strongly interacted with the Mpro target, emphasizing non-binding interactions as more crucial than hydrogen bonding in stabilizing the receptor-ligand conformation.

Presenter: Nguyen Quoc Thai

P.64 – Poster, VCTP-50

Thermal fluctuations and mass imbalance impacts on excitonic-polaritonic condensation in a microcavity

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Signatures of the excitonic-polaritonic condensates affected by thermal fluctuations in an electron-hole mass imbalance optical microcavity are inspected. In the framework of the unrestricted Hartree-Fock approximation, a two-band electronic model with mater-light coupling is solved and we find a set of self-consistent equations specifying the excitonic and photonic condensate order parameters. Numerical results reveal a complex competition between the instabilities of the excitonic, polaritonic and photonic condensation states under the influence of the electron-hole mass imbalance and the thermal fluctuations. The distinctive features of excitonic-polaritonic-photonic condensates are also characterized by the momentum distributions of the electron-hole pair amplitude and the photonic density.

Presenter: Do Thi Hong Hai

P.65 – Poster, VCTP-50

Molecular Simulation of Noble Gas Fractionation in CO_2-Water Systems under Geological Conditions

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Abstract: Understanding the fractionation of noble gases in CO_2-H_2O equilibrium systems is crucial for their application as geochemical tracers in geological carbon storage and subsurface fluid processes [1]. However, both accurate data and a comprehensive molecular-level understanding of noble gas partitioning under relevant geological conditions remain limited [2]. In this study, we investigate the equilibrium fractionation of noble gases between CO_2 and water phases using Gibbs ensemble Monte Carlo (GEMC) simulations, combined with the continuous fractional component approach [3]. Carbon-dioxide, water, and noble gases (He, Ne, Ar, Kr, Xe) molecules are described using the TraPPE, TIP4P/2005, and spherical Lennard-Jones force fields, respectively [4-6]. Unlike interaction parameters are systematically adjusted to reproduce available experimental solubility data [2, 3]. Extensive GEMC simulations are performed over a wide range of thermodynamic conditions relevant to deep subsurface reservoirs. We systematically analyze effects of temperature and pressure on noble gas fractionation induced by solubility, providing molecular-level insight into partitioning processes in CO_2-H_2O equilibrium systems.

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Presenter: Nguyen Tu Khai Nam

P.66 – Poster, VCTP-50

Interfacial Tension of Carbon Dioxide – Water: A Molecular Simulation Study

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The interfacial tension (IFT) between CO_2 and water plays a key role in governing capillary trapping, fluid migration, and plume stability during subsurface CO_2 storage and utilization processes [1]. Accurate prediction of CO_2-water IFT is essential for modeling multiphase flow in porous media and assessing storage security. In this study, molecular dynamics (MD) simulations are employed to compute CO_2-water IFT over a wide range of thermodynamic conditions. The TraPPE force field is used to model CO_2, and the TIP4P/2005 model is adopted for water, as these force fields are known to reproduce the thermophysical properties of pure phases with high accuracy [2-3]. The unlike interaction parameters are adjusted to match experimental Henry's law constant of CO_2 in water [4]. The dependence of IFT on temperature and pressure is analyzed, particularly across the critical point of CO_2 [5]. In addition, the simulation results are employed to verify scaling laws for the IFT.

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Presenter: Nguyen Ngoc Mai Phuong

P.67 – Poster, VCTP-50

Influence of Parameters on Structure, Phase Transitions, and Crystallization Processes of NiMn Alloys

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In this study, we examine the influence of heating rate, atomic numbers, annealing time, and temperature on the structure, phase transitions and crystallization processes of NiMn alloys using molecular dynamics simulations with periodic boundary conditions. The structural characteristics, phase transition, and crystallization behavior are quantitatively evaluated using several analytical approaches, including the radial distribution function (RDF), total system energy (Etot), particle size (D), and Common Neighborhood Analysis (CNA). Changes in structural unit distributions—such as Face-Centered Cubic (FCC), Hexagonal Close-Packed (HCP), Body-Centered Cubic (BCC), and Other phases—are observed in response to variations in input parameters.

Presenter: Mai Van Dung

P.68 – Poster, VCTP-50

First-principles insights into electron–phonon scattering limited mobility in two-dimensional Janus materials

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Two-dimensional (2D) materials are emerging as key candidates for next-generation electronic devices. To assess their application potential, it's crucial to accurately determine their carrier mobility, which is governed by electron-phonon scattering processes. Our research utilizes density functional theory (DFT) calculations to determine carrier mobility in several 2D Janus materials, taking into account various phonon scattering mechanisms. We have successfully identified the dominant scattering mechanisms that significantly impact mobility, thereby shedding light on the electronic transport characteristics of these materials.

Presenter: Nguyễn Ngọc Hiếu

P.69 – Poster, VCTP-50

BCS–BEC crossover of the equilibrium excitonic-polaritonic condensates in the mass imbalance optical microcavities

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Electron-hole mass imbalance and Coulomb interaction impacts on the BCS–BEC crossover of

the excitonic-polaritonic condensation states in the equilibrium optical semiconducting microcavities are examined. Within the unrestricted Hartree–Fock framework applied to a two-band electronic system incorporating both the electron–hole Coulomb attraction and light–matter coupling on an equal footing, the polaritonic condensate order parameter is selfconsistently solved. The excitonic and photonic susceptibilities evaluated by the random phase approximation specify the phase boundaries of the excitonic-polaritonic-photonic condensate structures. Analyzing the momentum distributions of the electron-hole pair amplitude and photonic density shows us the complex BCS-BEC crossover of the condensation states. The phase diagram indicates significant roles of the Coulomb interaction and mass imbalance on the stabilities of the excitonic-polaritonic condensation states in the equilibrium optical microcavities.

Presenter: Nguyen Thi Hau

P.70 – Poster, VCTP-50

Impact of laser parameters on photoisomerization probability in hydrogen cyanide

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Laser-driven control of the isomerization process of the hydrogen cyanide (HCN) molecule has attracted attention due to its potential to enhance the formation yield of HNC isomer. Previous studies showed that two-color lasers – combinations of two lasers with different frequencies, can significantly enhance the isomerization probability compared with one-color laser. However, the influence of individual laser parameters remains insufficiently explored. In this study, we extend the investigation to clarify the influence of various laser parameters on the isomerization probability. Specifically, we examine the effects of intensity, pulse duration, and direction of laser polarization for one-color laser, and of intensity and relative phase for two-color lasers. To simulate the interaction of the HCN molecule with a laser field, we firstly calculate the potential energy surface (PES) using the Complete Active Space Self-Consistent Field method via the ORCA program. The isomerism process is simulated by numerically solving the time-dependent Schrödinger equation for the motion of hydrogen nucleus in the effective potential of PES and laser-molecular dipole coupling. The results reveal the specific regions of laser parameters for optimizing the isomerization probability. Remarkably, in high-probability cases, we observe the tunneling and interference effects in the nuclear wavefunction. The project is ongoing with indication of these effects in measurable signals.

Presenter: Lê Viết Nam

P.71 – Poster, VCTP-50

Study and design organic semiconductor materials with outstanding properties using New quantum computing methods

Tran Tri Nhan, Tran Nguyen Lan

VNUHCM - University Of Science,

In the field of organic light-emitting diodes (OLEDs), the recombination of charge carriers gen-

erates singlet and triplet excited states in a 1:3 ratio. Triplet states typically do not emit light due to spin-forbidden transitions, resulting in energy loss and reduced luminescence efficiency. Designing organic materials with an inverted singlet–triplet gap (INVEST) can enhance emission efficiency and device stability. However, accurately predicting these properties requires computational methods that are both highly accurate and cost-effective. In this study, we improve and apply the O2BMP2 method — a novel computational approach that incorporates two-particle correlation within a one-particle framework — to predict singlet–triplet energy gaps and assist in the design of INVEST materials. This method significantly reduces computational complexity from $O(N^5)$ to $O(N^4)$, making it suitable for large-scale materials screening. Our results contribute not only to the development of efficient simulation tools but also to new directions in designing next-generation emissive materials for OLED technologies.

Presenter: Trần Trí Nhân

P.72 – Poster, VCTP-50

Scoto-seesaw model implied by flavor-dependent Abelian gauge charge

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Assuming fundamental fermions possess a new Abelian gauge charge that depends on flavors of both quark and lepton, we obtain a simple extension of the Standard Model, which reveals some new physics insights. The new gauge charge anomaly cancellation not only explains the existence of just three fermion generations as observed but also requires the presence of a unique right-handed neutrino ν_R with a non-zero new gauge charge. Further, the new gauge charge breaking supplies a residual matter parity, under which the fundamental fermions and ν_R are even, whereas a right-handed neutrino N_R without the new charge is odd. Consequently, light neutrino masses in our model are generated from the tree-level type-I seesaw mechanism induced by ν_R and from the one-loop scotogenic contribution accommodated by potential dark matter candidates, N_R and dark scalars, odd under the matter parity. We examine new physics phenomena related to the additional gauge boson, which could be observed at colliders. We analyze the constraints imposed on our model by current experimental limits on neutrino masses, neutral meson oscillations, B-meson decays, and charged lepton flavor violating processes. We also investigate the potential dark matter candidates by considering relic density and direct detection.

Presenter: Nguyen Tuan Duy

P.73 – Poster, VCTP-50

Entanglement dynamics of an atom interacting with a generalized photon-added pair coherent state under phase damping

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(2) Department of Physics, University of Education, Hue University, Hue City, Vietnam

In this paper, we investigate the entanglement dynamics of a two-level atom interacting with a field initially prepared in a generalized photon-added pair coherent state under the influence

of phase damping. We analyze how entanglement evolves over time and how it is affected by the photon addition numbers and the strength of decoherence. Special emphasis is placed on comparing the behavior of entanglement when the field is in a superposition of a photon-added pair coherent state. Our results show that the superposed states exhibit enhanced entanglement robustness under phase damping, particularly in the early evolution stages. These findings suggest that engineering initial field states through photon addition and quantum superposition can significantly influence entanglement preservation. The results have potential applications in quantum information processing, where maintaining entanglement under noise is essential.

Presenter: Le Thi Hong Thanh

P.74 – Poster, VCTP-50

Tracking nuclear vibration using mass spectrometry

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Tracking ultrafast molecular motion is a fundamental prerequisite for gaining control over quantum processes. One effective way for tracking ultrafast molecular motion is the pump–probe technique, in which an initial pump pulse excites nuclear dynamics, followed by a delayed probe pulse that triggers the fragmentation of molecule - which is known as Coulomb Explosion (CE) [1]. By using mass spectrometry, the ionic signals from the molecule are analyzed to obtain the distribution of fragments versus their kinetic energy, or shortly the Kinetic Energy Release (KER) spectra, which encode nuclear dynamics at the instant CE occurs [1,2]. In this study, we theoretically study the posibility of tracking nuclear vibrations of the ion $H_2{}^{2+}$; in which, the KER spectrum is considered to be contributed mostly by fragments from molecule in two lowest electronic states. By analyzing KER spectra as a function of the time delay between pump and probe pulses, the frequencies of nuclear vibration are extracted via Fourier transform [3]. The results are consistent with previous studies and demonstrate the potential of Coulomb Explosion as an effective tool for probing ultrafast nuclear dynamics [4]. The project is ongoing, aiming to track the nuclear dynamics of more complex molecular systems or those driven by multiple input laser pulses.

Keywords: Mass Spectrometry, Coulomb Explosion, Kinetic Energy Release.

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Presenter: Nguyen Dang Trong Thanh

P.75 – Poster, VCTP-50

Analytical method: Universal formula for obtaining fundamental material parameters of monolayer transition metal dichalcogenides from experimental exciton energies

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Monolayer transition metal dichalcogenides (TMDCs) have attracted much research attention because their high binding energies. Exciton, excited bound electron-hole pairs, have been found and studied in this material. Experiments show that the exciton binding energy strongly depends on material parameters such as: reduced exciton mass, polarizability, and dielectric constant of the surrounding medium. This suggests to us a method to extract information about materials from their experimental energy spectra. Based on the analytical expressions already developed for this type of material with a large range of material parameters, we construct a universal formula to extract material parameters straightforward and highly accurate from experimental energy spectra. By applying this method, we extract material parameters E_g, r_0, μ and κ from the magnetoexciton energies of monolayer TMDCs encapsulated by different in various current experiments

Presenter: Lê Hoàng Việt

P.76 – Poster, VCTP-50

Unraveling the electronic mechanisms of transition metal and fluorine codoping for enhanced electrochemical performance in sodium lithium manganese oxide cathodes

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Enhancing the structural stability and electronic and electrochemical properties of sodium-ion cathode materials is essential for developing the next generation of sodium-ion batteries. In this study, we carry out first-principles calculations to assess the performance of P2-type sodium lithium manganese oxide (NLM) cathodes co-doped with transition metals X (X = Sc, Ti, V, Cr, Fe, Co, Ni, Cu, and Zn) and fluorine. Our findings reveal that among the investigated transition metals and fluorine, codoping cobalt and fluorine atoms helps mitigate Jahn-Teller distortions, thus stabilizing the NLM cathodes. The stability of this most promising cobalt-fluorine co-doped heterostructure is further validated by experimental X-ray diffraction patterns synthesized by the standard sol-gel method. Regarding electronic properties, the pristine NLM systems exhibit ferromagnetic metallic behavior. However, cobalt-fluorine co-doped systems display ferromagnetic semi-metallic characteristics, featuring a mix of free holes and electrons. The doped system shows a higher carrier density and lower activation energies, leading to improved transport prop-

erties compared to the undoped systems. These results highlight the significant role of co-doping cobalt and fluorine atoms in creating high-performance sodium-ion cathodes.

Presenter: Nguyen Chi Ben

P.77 – Poster, VCTP-50

A geometrical model for protein folding with directional interactions

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Alpha-helices and beta-sheets are repetitive protein secondary structures stabilized by hydrogen bonding, the steric constraints of the polypeptide chain and also hydrophobic interactions specified by the amino acid sequence. Studies have shown that these structures can arise from simple geometrical considerations of a tube-like homopolymer represented by a chain of cylindrical discs or coins. Here, we develop a polymer model based on a chain of spherical beads, incorporating the geometrical constraints on local conformations of residues that form hydrogen bonds and directional poking contact interactions. Our model demonstrates that protein-like structures can emerge on the basis of these considerations. The model also yields a free-energy landscape with relatively few broad minima even for a homopolymer, consistent with the fact that proteins can be designed to enable rapid folding to their native states.

Presenter: Trinh Xuan Hoang

P.78 – Poster, VCTP-50

Study of Neutrino Masses from an A_4-Based Seesaw Model

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(2) International Centre for Interdisciplinary Science and Education (ICISE)

In this study, we investigate the origin of neutrino masses and the mechanism of CP violation in the lepton sector by constructing a Standard Model extension based on the discrete non-Abelian flavor symmetry group $\mathbf{A}_4$. The model introduces three generations of right-handed neutrinos and an extended scalar sector composed of one A_4 triplet Higgs and three scalar singlets, allowing for a realistic mass structure in the lepton sector.

Neutrino masses are generated via a **Type-I Seesaw mechanism**, with the Dirac and Majorana mass matrices derived explicitly from the model's Yukawa Lagrangian. Perturbative analysis around the tribimaximal (TBM) mixing limit is performed, introducing small corrections through symmetry-breaking parameters ϵ_+ and ϵ_-. Analytical expressions for neutrino mass eigenvalues, mixing angles, and the Dirac CP phase δ_{CP} are obtained in terms of model parameters.

The model successfully predicts:

- Neutrino mass spectrum in the normal ordering with m_1, m_2, m_3 at eV level,
- The sum of neutrino masses $\sum m_\nu < 0.12\,\text{eV}$, consistent with cosmological bounds,
- An effective neutrino mass in beta decay $m_\beta \approx 0.010\,\text{eV}$,
- An effective Majorana mass for neutrinoless double beta decay $m_{\beta\beta} \approx 2.9\,\text{meV}$,

- A maximum Jarlskog invariant $|J_{CP}^{\max}| \approx 0.02$, compatible with current experimental ranges.

The model also establishes predictive sum rules relating mass eigenstates and provides analytical constraints on the Dirac CP phase using modified PMNS matrix elements. The results show good agreement with recent neutrino oscillation data and offer a compelling framework for interpreting future experimental results, especially from precision measurements of CP violation and rare lepton-number-violating processes.

Presenter: Tran Tien Manh

P.79 – Poster, VCTP-50

Effect of polarized light and magnetic field on the transport properties of germanene

Do Muoi

Faculty of Natural Sciences, Pham Van Dong University, Quang Ngai, VietNam

We present a theoretical study of quantum transport in germanene, a topological insulator under the influence of a perpendicular magnetic field and circularly polarized light. The interplay between the magnetic field and polarized light modulates the resulting band structure, while the topological characteristics are governed by low-energy surface state dynamics. Our results reveal the emergence of a novel quantum Hall state, in which the zeroth Landau level undergoes a quantum phase transition from a trivial insulating state with zero Hall conductivity at the charge neutrality point to a Hall insulating state characterized by a quantized Hall conductivity of e^2/h. These findings highlight the promise of germanene in next generation spintronic devices and open new experimental avenues for the exploration of unconventional quantum Hall states.

Presenter: Do Muoi

P.80 – Poster, VCTP-50

Enhanced Gas Sensing Performance via Au and B Co-doped Silicene/MoS2 Bilayer Heterostructures: A First-Principles Insight

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The development of highly sensitive and selective gas sensors remains a significant challenge in environmental monitoring and industrial safety. This study presents a comprehensive first-principles investigation of gold (Au) and boron (B) doped silicene/MoS2 bilayer heterostructures for enhanced gas sensing performance toward CO and CO2 detection. Using density functional theory (DFT) and non-equilibrium Green's function (NEGF) methodologies, we systematically explore the structural stability, electronic properties, adsorption mechanisms, and electron trans-

port characteristics of pristine and doped heterostructures. Our results indicate that Au and B doping substantially modifies the electronic structure, transitioning from semiconducting to metallic, thereby enhancing the sensitivity and responsiveness of the sensor through improved electron transfer and adsorption strength. Notably, the co-doped Au-B configuration demonstrates optimal sensing performance, characterized by significant adsorption energy, rapid recovery times, and pronounced charge transfer upon gas adsorption. These findings offer critical insights into atomic-scale interactions and present a viable strategy for designing advanced 2D material-based gas sensors with exceptional sensitivity and selectivity.

Presenter: Duong Trong Nhan

P.81 – Poster, VCTP-50

Control of Superconducting Qubits

Nguyen Van Duy

Phenikaa University

In superconducting quantum computing, precise control of qubit dynamics is crucial for achieving high-fidelity gate operations. One of the key challenges arises from the multilevel nature of transmon qubits, which can lead to leakage out of the computational subspace. To address this issue, the derivative removal by adiabatic gate (DRAG) technique has been proposed and extensively studied. In this presentation, we provide a theoretical overview of the DRAG method and its extensions to both qubit and qutrit systems. We show how properly shaped control pulses, including derivative components, can effectively suppress leakage and phase errors during gate implementation.

Presenter: Nguyen Van Duy

P.82 – Poster, VCTP-50

Reaching High Accuracy for Energetic Properties at Second-Order Perturbation Cost by Merging Self-Consistency and Spin-Opposite Scaling

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(2) Graduate University of Science & technology - Vietnam Academy of Science and Technology;
(3) University of Science, Vietnam National University, Ho Chi Minh City

Quantum chemical methods dealing with challenging systems while retaining low computational costs have attracted attention. In particular, many efforts have been devoted to developing new methods based on second-order perturbation that may be the simplest correlated method beyond Hartree-Fock. We have recently developed a self-consistent perturbation theory named one-body Møller-Plesset secondorder perturbation theory (OBMP2) and shown that it can resolve issues caused by the noniterative nature of standard perturbation theory. In this work, we extend the method by introducing spin-opposite scaling to the double-excitation amplitudes, resulting in the O2BMP2 method. We assess the O2BMP2 performance on the triple-bond N2 dissociation, singlet-triplet gaps, and ionization potentials. O2BMP2 performs much better than standard MP2 and reaches the accuracy of coupled-cluster methods in all cases considered in this work.

Presenter: Nguyen Thanh Hoang

P.83 – Poster, VCTP-50

Electric field enhances the electronic and diffusion properties of penta-graphene nanoribbon anodes in lithium-ion batteries

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(2) Faculty of Fundamental Sciences, Hanoi University of Industry;
(3) Department of Physics Education, Can Tho University

Enhancement of the ionic conductivity and reduction of diffusion barriers of lithium-ion batteries are crucial for improving the performance of the fast-growing energy storage devices. Recently, the fast-charging capability of commercial-like lithium-ion anodes with the smallest modification of the current manufacturing technology has been of great interest. We used first principles methods computations with density functional theory and the climbing image-nudged elastic band method to evaluate the impact of an external electric field on the stability, electronic band gap, ionic conductivity, and lithiumion diffusion coefficient of penta-graphene nanoribbons upon lithium adsorption. By adsorbing a lithium atom, these semiconductor nanoribbons become metal with a formation energy of -0.22 eV, and an applied electric field perpendicular to the surface of these nanoribbons further stabilizes the structure of these lithium-ion systems. Using the Nernst–Einstein relation, in the absence of an electric field, the ionic conductivity of these penta-graphene nanoribbons amounts to 1.24 $\times 10^{-4}$ S cm^{-}1. In the presence of an electric field, this conductivity can reach a maximum value of 8.89 $\times 10^{-2}$ S cm^{-1}, emphasizing the promising role of an electric field for supporting fast-charging capability. Our results highlight the role of an external electric field as a novel switch to improve the efficiency of lithium-ion batteries with penta-graphene nanoribbon electrodes and open a new horizon for the use of pentagonal materials as anode materials in the lithium-ion battery industry.

Presenter: Nguyen Vo Anh Duy

P.84 – Poster, VCTP-50

Probing charge migration of molecular ion from high-harmonic spectra

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(2) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 700000, Vietnam;
(3) Simulation in Materials Science Research Group, Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Vietnam

Attosecond physics is a pioneering field that explores ultrafast dynamics at the attosecond timescale, particularly the motion of electrons in atoms and molecules [1]. A phenomenon of interest is charge migration (CM), which refers to the temporal change in electron density within excited molecules [1]. Investigating CM is highly significant for understanding and controlling chemical reactions, offering the potential to enhance reaction efficiency and reveal novel reaction mechanisms [1].

To probe this ultrafast electron dynamic, high-harmonic generation (HHG) spectra emerge as a powerful tool [2-4]. The mechanism of HHG signal emission is described by the semiclassical three-step model, where an electron is ionized, propagates in the laser field, and recombines with the parent ion, emitting an HHG signal [8]. The next recombination takes place after a

few attoseconds, emitting another HHG signal [2]. These signals encode image of the ion at the moment of recombination [3]. By analyzing the attosecond-scale HHG signals emitted, we reconstruct the attosecond-resolution "movies" of electron density in molecular ions, enabling direct observation of charge migration [2-4].

While the CM reconstruction method from HHG spectra has been applied to various molecular ion [2-4], their quantitative accuracy remains uncharacterized. In this study, we implement this approach on carbonyl sulfide ion (OCS) - a previously unexplored target for CM studies, in which, the measured HHG spectra are considered as single-molecule response. In our results, we successfully reconstruct the CM of OCS from HHG spectra and validate the accuracy method against TDDFT simulation. The reconstructed CM shows excellent agreement with theoretical predictions, quantitatively confirming the method's is under 20% error. The project is ongoing, aiming to probe CM of OCS from HHG spectra of a gaseous sample of OCS molecule.

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Presenter: Nguyen Thanh Dinh Duy

P.85 – Poster, VCTP-50

Study of a single oxygen adatom on graphene using density functional theory

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In this talk, we will present a density-functional-theory study of a single oxygen adatom adsorbed on graphene lattice. We investigate all possible positions of the oxygen adatom so as to understand the structural stability, the density of states and the bonding characteristics of the adatom to the host lattice. We also consider the phonon spectra for each structural configuration in order to estimate the phonon-contributed free energy at high temperatures. Our study confirms the ground state structure of the oxygen-graphene structure and exhibits all possibile structures at high temperatures as well as the possibilities for the oxygen adatom to react with other substances. The results may be useful to understand some experiments for depositing atomic layers on the graphene lattice using oxygen.

Presenter: Tạ Văn Nam

P.86 – Poster, VCTP-50

Enhance sampling of amyloid beta peptide: the combination of molecular dynamics simulations and machine learning

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Molecular dynamics (MD) simulations are powerful and widely used tools for studying protein structure and function. However, conventional MD simulations often require extensive computational time to sufficiently sample the conformational space. To address this limitation, various enhanced sampling techniques such as replica exchange, umbrella sampling, and metadynamics have been developed. In this study, we combine molecular dynamics simulations with machine learning to explore the conformational space of the amyloid beta protein, both in its full-length form and in a truncated segment (residues 18–28). Specifically, we employ an autoencoder to project MD-generated conformations onto a low-dimensional conformational landscape defined by principal component analysis (PCA). Our results demonstrate that this integrated approach can serve as a useful predictive tool for identifying low-energy conformations of proteins amyloid beta and offers a promising alternative for enhanced sampling in MD simulations.

Presenter: Tran Thi Minh Thu

P.87 – Poster, VCTP-50

Unveiling HCN Isomerization Through HHG Spectrum Simulation

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High-order harmonic generation (HHG) is a highly nonlinear optical process that allows for the transformation of intense laser light into much shorter wavelengths. The HHG signal itself offers valuable insights into the electronic structure and dynamics of the material being studied. Thus, HHG spectroscopy is a versatile tool, applicable to a wide range of samples including atoms, molecules, solids, and even liquids. This work investigates the HHG of several molecular structures using the SLIMP (Strong Laser Interaction Model Package). The considered molecules involve hydrogen cyanide (HCN), hydrogen isocyanide (HNC), the transition state (TS), and various geometries found along the intrinsic reaction coordinate of HCN isomerization. The HCN, HNC, and TS were optimized at the MP2/6-311+G(d,p) level of theory. The HHG spectrum simulation was performed aiming to gain better insights into the HCN isomerization process. The so-obtained even-to-odd intensity ratio from HHG spectra will also be compared.

Presenter: Huỳnh Thị Hải

P.88 – Poster, VCTP-50

Research on stable phases in theoretical models for kagome magnetic materials.

Tran Thi Thanh Mai, Tran Minh Tien

Institute of Physics

We study the emergence and properties of stable phases in models of kagome magnetic materials. In previous work, we constructed a minimal model consisting of two key terms. The first term describes Heisenberg spin exchange between electrons. In this term, we consider the exchange to be isotropic within the plane but anisotropic out of plane. The second term represents the Dzyaloshinskii-Moriya interaction, which we assume to be aligned along the z-axis due to the symmetry of the kagome lattice. In this study, we extend the previous model to investigate magnetic competition in kagome magnetic systems. This extended model is based on a combination of the tight-binding model and the double exchange model. Using the Bogoliubov variational principle, we determine the ground state at zero temperature.

Presenter: Tran Thị Thanh Mai

P.89 – Poster, VCTP-50

Preliminary study of the correlation effects of a twisted bilayer structure of transition metal dichalcogenides

Son Trong Nguyen, Hung T. Dang

Faculty of Materials Science and Engineering, Phenikaa University

Twisted bilayer of transition metal dichalcogenides (tTMD) is a new generation of materials for studying strong correlation effects. Similar to twisted bilayer graphene at certain "magic" angles, the low energy electronic structure of tTMD may exhibit extremely narrow bands (flat bands), allowing for significant many-body effects. However, unlike graphene, tTMD may have such flat bands for a wider range of twisted angle, making it accessible for both experimentalists and theorists for investigation. Together with the easy tuning of the electron occupation via the gate voltage, tTMD is considered as a new kind of quantum simulator for studying strongly correlated systems. In this study, we conduct a preliminary theoretical study of a low-energy topologically-trivial Hubbard model of a twisted bilayer structure of triangular TMDs (such as WS_2, WSe_2, hBN) using single-site dynamical mean-field theory. We discuss all possible aspects of strong correlation in this model, such as the mass enhancement, the Mott transition and the formation of magnetic order at low temperatures. This study will be the starting point for studying other more complicated structures in the family of tTMDs.

Presenter: Nguyen Trong Son

P.90 – Poster, VCTP-50

Polarized ZZ pair production at the LHC: Theoretical status

Duc Ninh Le, Thi Nhung Dao

Phenikaa University, Hanoi, Vietnam

In this presentation, we provide an overview of the theoretical status of polarized ZZ pair production at the LHC, with fully leptonic decays. The state-of-the-art prediction includes next-to-next-to-leading order QCD corrections, next-to-leading order electroweak corrections, and parton shower effects. Corresponding distributions from the latest ATLAS simulation will be presented for the sake of comparison. This remarkable result has been recently achieved via a collective effort of theorists and experimentalists working on polarized ZZ pair production at the LHC across the globe (arXiv:2505.09686).

Presenter: Le Duc Ninh

P.91 – Poster, VCTP-50

Anharmonic high-order XAFS cumulants of crystalline silver within quantum-statistical perturbation theory

Le Viet Hoang (1), Tong Sy Tien (2), Nguyen Thi Minh Thuy (2,3), Nguyen Huy Thao (3), Nguyen To Nu (3), Nguyen Cong Toan (1)

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(3) Hanoi Pedagogical University 2

The anharmonic high-order X-ray absorption fine structure (XAFS) cumulants of crystalline silver (Ag) have been theoretically analyzed with explicit consideration of thermal disorder effects. The proposed model is formulated based on the first-order perturbation approach within the framework of quantum statistical theory, incorporating the correlated Einstein model and an anharmonic effective potential that characterizes atomic interactions. The resulting thermodynamic XAFS parameters account for both atomic correlation and anharmonicity, explicitly including the influence of nearest-neighbor atoms on the absorber and backscatter. The temperature-dependent expressions are derived in explicit analytical form, accurately describing the physical behavior in both low- and high-temperature regimes. Numerical calculations for Ag exhibit good agreement with available experimental data and other theoretical models throughout the temperature range of 0–1000 K. These results confirm that the present theoretical framework is effective for analyzing anharmonic high-order XAFS cumulants in thermally disordered metals, particularly those exhibiting complex thermal dynamics. Keywords: Anharmonic high-order XAFS cumulants, crystalline silver, quantum-statistical perturbation theory, thermal disorder

Presenter: Lê Việt Hoàng

P.92 – Poster, VCTP-50

Phase diagram for the pseudogap Kondo effect in graphene

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Adatoms placed on graphene is a potential direction for investigation in condensed matter physics and materials science. The fundamental problem in this topic is to understand how the Kondo effect exhibits in this system, i.e. how electrons from the graphene screens the impurity. With its linear energy dispersion, graphene can be a potential host material to realize the pseudogap Kondo effect where there is a quantum phase transition from the Kondo screening phase to impurity free local moment. In this work, the full phase diagram for such phase transition is presented, showing linear relation between the electron correlation strength and the impurity energy level at criticality and the nonlinear behavior of the phase boundary with respect to the hybridization between the graphene sheet and the impurity. Detailed analysis shows the important role of the impurity occupancy, which can be used to interpret the behaviors of the phase diagram.

Presenter: Dang The Hung

P.93 – Poster, VCTP-50

Effect of dynamic core-electron polarization on High-order harmonic generation from oriented co molecules

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Previous research on the effect of dynamic core-electron polarization (DCEP) [1] on high-order harmonic generation (HHG) from CO molecules mostly focused on the parallel orientation (0○), where the molecular axis aligns with the laser polarization [2]. While other works extended the analysis to other orientations, they were limited to only a few representative harmonic orders [3]. A recent study on the 70° orientation revealed notable differences in DCEP effects compared to the parallel case [4], suggesting the orientation-dependent behavior of DCEP effect. Motivated by these findings, this study provides a more comprehensive understanding by investigating the effect of DCEP on the full HHG spectrum across a broad range of orientation angles. To calculate the HHG spectra from CO molecules, we numerically solve the time-dependent Schrödinger equation (TDSE) within the Single-Active Electron (SAE) approximation, incorporating the DCEP potential. The results show that the molecular orientation with respect to the laser polarization strongly impacts the manifestation of DCEP in HHG spectrum, as reflected in the intensity ratio of even harmonics to the two adjacent odd ones, which characterizes the intrinsic asymmetry of the molecule [2]. The time-frequency analysis for HHG emission also provides evidence for the effects of DCEP in the time domain, particularly through the modification in intensity and phase of HHG signals emitted every half cycle of the laser.

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Presenter: Dam My Hoa

P.94 – Poster, VCTP-50

Multielectron Effects in the High-Order Harmonic Generation Spectrum of Magnesium

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Multielectron effects are critical for accurately modeling the interaction between atoms and intense laser pulses. While the single active electron (SAE) approximation considers only the outermost electron to be active, multielectron effects can be understood as the interaction between the active electron and the laser-induced dipole of the remaining electrons in the ion – a phenomenon known as multielectron polarization (MEP). Accordingly, MEP is expected to exhibit significant effects in targets with high polarizability. In this work, we investigate the influence of MEP on the high-order harmonic generation (HHG) spectrum of the magnesium atom, which has a relatively simple electronic structure and a highly polarizable ionic core. By solving the time-dependent Schrödinger equation (TDSE) for the active electron both with and without the MEP, we show that increasing the laser intensity leads to the enhancement of intensity in the near-cutoff region of the HHG spectrum. By analyzing ionization rates and HHG time profiles, we figure out that this enhancement is attributed to the suppression of laser-induced ionization and the increase in the recombination probability. Furthermore, MEP is observed to shift the HHG emission time to earlier moments compared to the case without MEP. These findings underscore the importance of incorporating MEP in strong-field simulations and suggest extending such studies to atoms with highly polarizable cores and under varied laser parameters to fully characterize MEP's role in HHG.

Presenter: Lê Trần Nhật Hào

P.95 – Poster, VCTP-50

Constrain the free parameters of Lepton Flavor Symmetry Models with Neutrino Oscillation data

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Lepton flavor models stemming from discrete non-Abelian flavor symmetries, characterized by free model parameters, successfully provide specific predictions for some of the leptonic mixing angles and the Dirac CP-violating phase. They also predict the existence of algebraic relations among certain mixing parameters, commonly referred to as sum rules. In our previous work (https://doi.org/10.1103/PhysRevD.111.073003), we investigated the possibility of testing these lepton flavor models via the solar and atmospheric sum rules, which describe the predictability of the less-known δ_{CP} based on its relationship with other more precisely constrained mixing angles $(\theta_{12}, \theta_{13}, \theta_{23})$, using their current constraint from the global neutrino data. In this study, we develop a new framework that enables us to test these models by directly constraining their free parameters using experimental data from neutrino oscillation experiments. The preliminary results show that the allowed ranges and the precision of the leptonic mixing angles are crucial for confirming or excluding specific flavor models. Data from two forthcoming, large-scale, accelerator-based long-baseline neutrino experiments, Hyper-Kamiokande (T2HK), and the Deep Underground Neutrino Experiment (DUNE) as well as possible joint analyses from future neutrino facilities, will allow us to exclude certain models in specific regions of both the

standard oscillation parameter space and the model parameter space.

Presenter: Phan To Quyen

P.96 – Poster, VCTP-50

Population imbalance driven Mott transitions in three-component Falicov-Kimball model

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Population imbalance driven Metal-insulator transitions of a three-component Falicov-Kimball model are investigated within Kotliar-Ruckenstein mean-field slave boson approach. Although the main results have been obtained within the saddle point slave-boson approach, their qualitative features are in good agreement with those obtained by the dynamical mean-field theory. Therefore, we believe that the slave-boson technique is a good commentary and/or alternative approach for more complex ultracold atom mixtures where the application of the dynamical mean-field theory is not realizable.

Presenter: Tran Minh Tien

P.97 – Poster, VCTP-50

Statistical Analysis of Score Distribution Transitions in Non-Centralized Assessments: A Case Study of Final Exam

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Data from the Hanoi Department of Education and Training reveal concerning trends in the results of the 12th-grade student quality assessment conducted in March 2025. Notably, 6.78% of students scored below 3 out of 10, with 0.91% receiving critically low scores of 1 or less—placing them at significant risk of being ineligible for graduation without substantial improvement in the official final exam. Furthermore, 32% of students scored below average (under 5 points), highlighting widespread academic underperformance. Among all subjects, Mathematics recorded the highest rate of below-average scores (51.69%), followed closely by Geography (51.42%) and Biology (50.41%). These results contrast sharply with data from the 2020 national high school exam, where Mathematics and Physics had the highest mean scores, while English had the lowest ones. Interestingly, Biology scores exhibit a near-normal distribution, suggesting underlying stability in assessment or instruction in that subject. This study applies statistical modeling techniques to investigate the transitions in score distributions across subjects, aiming to uncover the mechanisms behind these shifts. By analyzing structural and systemic factors influencing score variance, we propose an adjusted model to support fairer and more effective assessment design for future national examinations.

Presenter: Chu Thuy Anh

P.98 – Poster, VCTP-50

Developing an Interactive Computational Platform for Molecule-Surface Material Interaction: Applying to Area Selective Atomic Layer Deposition simulations

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Understanding molecule–surface interactions is critical for designing area-selective atomic layer deposition (AS-ALD) processes. While existing computational methods such as DFT or kinetic Monte Carlo offer valuable insights, they are often resource-intensive and not easily accessible. In this study, we address the need for a lightweight and user-friendly simulation tool by developing an interactive platform that models steric hindrance-based adsorption during AS-ALD. Drawing inspiration from previous Monte Carlo and random sequential adsorption studies, our platform allows users to simulate and visualize the adsorption of precursors and inhibitors on solid surfaces with adjustable molecular parameters. We demonstrate that molecular size, shape, and packing density significantly influence selective adsorption behavior. This platform provides an intuitive and efficient environment for exploring AS-ALD mechanisms, supporting both early-stage screening and educational use, and filling a methodological gap between high-fidelity modeling and experimental interpretation.

Presenter: Ngo Dang Huy

P.99 – Poster, VCTP-50

Dark matter relic abundance in an extended scalar sector with vector-like quarks

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This thesis investigates a minimal extension of the Standard Model (SM) that incorporates a Z_2-odd inert scalar doublet, a real singlet scalar, and vector-like quarks (VLQs). The model provides a viable candidate for scalar dark matter and allows for additional heavy scalar states that mix via a real orthogonal rotation. Only the SM Higgs doublet acquires a vacuum expectation value, preserving the Z_2 symmetry and ensuring dark matter stability. Particular attention is paid to the scalar sector, where mixing effects and CP assignments are carefully implemented. We classify all relevant interaction vertices and analyze dark sector phenomenology through scalar pair annihilation and co-annihilation processes into SM particles. We compute the squared matrix elements, perform interference analysis, and study resonance structures in the total annihilation cross section, using the standard freeze-out method to determine the relic abundance. Our results focus on identifying model configurations that yield a relic density compatible with observational data, thereby providing a robust foundation for further exploration of dark matter dynamics in extended scalar sectors.

Presenter: Nguyen Minh Hien

P.100 – Poster, VCTP-50

Investigation of the soft parameter in the electron-ion coulomb potential and the governing mechanisms of nonsequential triple ionization in noble gas atom

Chau Bao Khoa (1), Truong Dang Hoai Thu (1), Do Van Tai (1), Ho Nguyen Xuan Bach (1)*

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In this study, based on the three-dimensional classical ensemble model, we propose a procedure to determine the soft parameter in the Coulomb interaction potential between ionized electrons and the parent ion. This is an important parameter used in the simulations of nonsequential triple ionization (NSTI) of noble gas atoms. Two physical conditions are applied to constrain this parameter: ensuring that all three electrons consistently have positive kinetic energy and preventing the autoionization of the atom. In addition, we analyze the dominant mechanisms governing the ionization dynamics and validate the results by comparing the ionization probabilities and recoil ion momentum distributions with previous experimental and theoretical data.

Presenter: Chau Bao Khoa

P.101 – Poster, VCTP-50

Searching for carbon cluster isomers using machine-learning potential

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We utilize the recently developed machine-learning potential, namely GAP-20, to predict the low-energy isomers of twelve-atom C clusters. While the GAP-20 aligns well with density-functional theory calculations for most isomers, accurately describing geometric structures and average C-C bond lengths, it significantly underestimates energies related to cage-like structures, leading to incorrect ground state predictions. Notably, the Jahn-Teller distortion associated with monocyclic rings is absent. These intriguing findings prompt further investigation. Additionally, GAP-20 identifies two novel low-energy isomers composed of multicyclic rings, challenging our existing knowledge and opening exciting avenues for future research. Overall, GAP-20 provides valuable insights into the complex landscape of carbon clusters by illuminating these multicyclic configurations.

Presenter: Nguyen Duy Huy

P.102 – Poster, VCTP-50

Tripeptides inhibit dual targets AChE and BACE-1: a computational study

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Alzheimer's disease (AD) is a progressive neurodegenerative disorder characterized by cognitive decline and memory loss, with amyloid-beta (Aβ) plaques and acetylcholine deficits being central

pathological features. Inhibition of dual targets including acetylcholinesterase (AChE) and beta-site amyloid precursor protein cleaving enzyme 1 (BACE-1) represents a promising strategy to address cholinergic deficits and amyloid pathology. In this study, we used computational approaches to evaluate 8000 tripeptides as potential dual inhibitors of AChE and BACE-1. Machine learning models revealed the four top-lead tripeptides including WHM, HMW, WMH, and HWM. Molecular docking simulations indicated that WHM possessed the most favorable interactions through hydrogen bonds, $\pi-\pi$ stacking, and salt bridges with key catalytic residues in both enzymes. Molecular dynamics simulations confirmed the stability of the protein-ligand complexes, with WHM exhibiting the most consistent conformations and significant disruption of catalytic residue geometries. Free energy perturbation analysis further supported WHM's superior stability across both targets. ADMET predictions suggested moderate oral absorption and limited brain penetration, consistent with the typical behavior of peptide-based compounds. Overall, WHM demonstrated the strongest potential as a dual inhibitor of AChE and BACE-1, offering a promising lead for future therapeutic development in AD.

Presenter: Do Anh Tuan

P.103 – Poster, VCTP-50

An analytical approach to retrieving fundamental structural parameters of monolayer transition metal dichalcogenides from exciton spectra

Duy-Nhat Ly (1) and Van-Hoang Le (1)

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The bandgap, dielectric constant, and screening length are key parameters defining monolayer transition metal dichalcogenides' electronic and optical properties (TMDCs). Determining these parameters accurately is challenging, as it often requires complex and consuming computational methods or complicated experiments. This report presents an efficient analytical framework for retrieving these fundamental structural parameters from exciton energy spectra in a magnetic field. Based on recent work [1], where exact analytical expressions for exciton spectra were obtained, we derive analytical formulas for the bandgap, dielectric constant, and screening length from experimental exciton energies. The idea originates from solving the inverse problem (exciton energy spectra $\rightarrow$ fundamental structural parameters) —as proposed in our earlier work [2]. The analytical formulas presented here are validated against experimental data and show excellent agreement across various TMDC materials. Moreover, the method significantly reduces computational complexity by avoiding the simultaneous fitting of multiple parameters. A comparison with results based on the Rytova–Keldysh potential shows deviations within 1.0 meV, even in strong magnetic fields.

Presenter: Lý Duy Nhất

P.104 – Poster, VCTP-50

Influence of local deformation on the adsorption of toxic gases on MoS2 monolayer: a first-principles investigation

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This work explores the adsorption characteristics of gas molecules (CO, CO2, NH3) on monolayer MoS2, with particular attention to the impact of local structural deformation using density functional theory. Initial calculations reveal distinct preferential adsorption sites (top, bridge, and hollow) on pristine MoS2. Following structural optimization, the number and nature of stable adsorption sites significantly evolve, influenced by induced local surface deformation. Electronic structure analyses indicate that deformation not only alters site-specific adsorption energies but also enhances the molecule-substrate interaction, potentially improving gas-sensing capabilities of the MoS2 monolayer. The anticipated results suggest that controlled local deformation could serve as an effective strategy to tailor the sensitivity and selectivity of MoS2-based sensors for detecting CO, CO2, and NH3, providing insights for the practical application of two-dimensional materials in environmental sensing technologies.

Presenter: Vương Khiết An

P.105 – Poster, VCTP-50

Mechanical and electronic properties of TiVZrNbMox high entropy alloys: First principles calculations

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The TiVZrNbMo alloy, a lightweight high-entropy alloy, is distinguished by its exceptional mechanical properties and remarkable high-temperature stability. Modulating the concentration of constituent elements, particularly Mo, induces significant variations in the alloy's physical and chemical characteristics. In this study, we employ first-principles calculations to investigate the structural stability, mechanical properties, and electronic characteristics of the TiVZrNbMox (x = 0.25, 0.5, 0.75, 1.0, 1.5, 2.0) alloy, with x systematically varied. The results reveal that increasing Mo content leads to a gradual reduction in the lattice constant. The binding energy of the samples demonstrates high stability. Regarding mechanical properties, the incorporation of Mo significantly influences the elastic constants, bulk modulus, and anisotropy, as evaluated through the Young's modulus. By simulating the stress–strain relationship, we determine the ultimate tensile strength (UTS) of the alloy, highlighting its dependence on Mo concentration. In terms of electronic properties, analyses of the band structure and density of states (DOS) elucidate the pivotal role of Mo in modulating the electronic characteristics of the system. These findings provide profound insights into the interplay between chemical composition and the properties of high-entropy alloys, paving the way for the optimization of advanced materials tailored for high-technology applications.

Presenter: Huynh Khanh Van

P.106 – Poster, VCTP-50

Matching High Energy Scale Theory to Standard Model and Prediction of the Higgs Boson Mass

Dao Thi Nhung

Phenikaa University

In this presentation we present a matching method with two possible matching conditions to match a theory at high energy scale to the low energy theory which is assumed to be the SM. This method is then applied to predict the Higgs boson mass. We discuss also uncertainties related to each matching condition

Presenter: Dao Thi Nhung

P.107 – Poster, VCTP-50

Effects of laser parameters on orbital competition in high-order harmonic generation from hydrogen cyanide

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Recent advances in laser technology have led to the discovery of various strong-field nonlinear phenomena, such as above-threshold ionization (ATI), high-energy ATI (HATI), nonsequential double ionization (NSDI), and high-order harmonic generation (HHG). These effects enable ultrafast imaging and tracking of electronic dynamics in atoms and molecules, necessitating accurate theoretical models to interpret the underlying mechanisms. A widely used and computationally feasible approach involves solving the time-dependent Schrödinger equation (TDSE) within the single active electron (SAE) approximation. Prior studies often attribute HHG signals predominantly to the highest occupied molecular orbital (HOMO), while neglecting the role of lower-lying orbitals. However, emerging evidence reveals the significance of multielectron effects, notably the contribution of HOMO-1 and its interaction with HOMO, which can manifest as observable changes in HHG spectra. In this work, we investigate the multiorbital contributions to HHG in hydrogen cyanide (HCN) molecules, focusing on the competition between HOMO and HOMO-1 under varying laser parameters. By numerically solving the TDSE using an SAE model that incorporates the orbital energies and permanent dipoles of both orbitals, we systematically examine how pulse duration, intensity, and wavelength affect their respective contributions. Our results show that the dominance of HOMO or HOMO-1 is not fixed but varies strongly with laser intensity and pulse duration, while remaining comparatively stable with respect to wavelength. Specifically, longer pulses and higher intensities enhance the role of HOMO-1, leading to suppression of HOMO contributions and shaping the overall HHG spectrum. Time-frequency analyses of the harmonics reveal that these dependencies originate from differences in the ionization probabilities and recombination dipole moments of the orbitals under changing field conditions. These findings underscore the importance of laser parameter selection when using HHG to probe multielectron dynamics and inner-valence orbital effects in asymmetric molecules.

Presenter: Hoàng Trọng Đại Dương

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