Program & Abstracts

49th Vietnam Conference on Theoretical Physics

HỘI NGHỊ VẬT LÝ LÝ THUYẾT VIỆT NAM LẦN THỨ 49

Huế

30 July-2 August 2024

Program & Abstracts

49th Vietnam Conference on Theoretical Physics

Huong Giang Hotel
51 Le Loi Street,
Hue City, Vietnam

30 July-2 August, 2024

Contents

Welcome Message

It is a great pleasure to welcome you to the 49th Vietnam Conference on Theoretical Physics (VCTP-49).

The VCTP-49 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, a category 2 centre under the auspices of UNESCO. VCTP-49 is also sponsored by Asia Pacific Center for Theoretical Physics (APCTP).

The VCTP, formerly known as 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 121 participants. 12 invited talks, 17 oral and 71 poster contributions will be presented. In addition, there also will be an experimental satellite session for poster presentations of high school students.

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)
- Nguyen Tuan Duy (Institute of Physics, VAST)

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- Tran Thi Thanh Mai (Institute of Physics, VAST, Hanoi)
- 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-49 conference takes place in:

Huong Giang Hotel
51 Le Loi Street,
Hue City, 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 conference room on the fifth floor of the Huong Giang Hotel. Please follow the direction in the lobby to go to the conference room.

Lunches

Lunches are provided for conference participants in the Huong Giang 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: 1 August 2024, from 19:00 PM
Place: Riverside Restaurant, Huong Giang Hotel.

For your family members to attend the Gala Dinner, please buy tickets from the conference secretary on 30 July.

VTPS Meeting

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

Time: 17:45 PM - 18:30 PM, Tuesday, 30 July 2024.
Place: Conference room, fifth floor, Huong Giang Hotel.

VTPS Young Research Award

At the opening session of the conference there will be an announcement and the delivery of the 2024 VTPS Young Research Award.

Program timetable

Time	Tuesday, 30 July	Time	Wednesday, 31 August	Thursday, 1 August	Time	Friday, 2 August
08:30 – 10:00	Registration (8:30) Opening (9:00) VTPS Young Research Award Vo Khuong Dien (I.1) Photo Session *(Chair: Trần Minh Tiến)*	08:30 – 10:00	Poster Session 1 *(Chair: Trinh Xuan Hoang)*		08:30 – 10:00	Poster Session 2 *(Chair: Nguyen Hong Quang)*
10:00 – 10:30	Coffee break	10:00 – 10:30	Coffee break		10:00 – 10:30	Coffee break
10:30 – 12:15	Bum-Hoon Lee (I.13) Ki Seok Kim (I.2) Dang Minh Triet (O.2) *(Chair: Bach Thanh Cong)*	10:30 – 12:00	Tran Nguyen Lan (I.6) Doan-An Trieu (O.6) Duong D. Hoang-Trong (O.7) *(Chair: Hoang Ngoc Cam)*		10:30 – 12:00	Le Van Hoang (I.10) Nguyen Van Duy (O.11) Tran Cong Minh (O.12) *(Chair: Le Dinh)*
12:15 – 14:00	Lunch	12:00 – 14:00	Lunch	Excursion	12:00 – 14:00	Lunch
14:00 – 15:30	Do Thi Huong (I.3) Do Quoc Tuan (O.3) Tran Minh Hieu (O.4) *(Chair: Phung Van Dong)*	14:00 – 15:30	Nguyen Quang Hung (I.7) Le Duc Ninh (O.8) Ranjeet Kumar (O.9) *(Chair: Tran Hoai Nam)*		14:00 – 15:30	Hoang Ngọc Cam (I.11) Quang-Huy Ho (O.13) Hoang Hai (O.14) *(Chair: Phan Van Nham)*
15:30 – 16:00	Coffee break	15:30 – 16:00	Coffee break		15:30 – 16:00	Coffee break
16:00 – 17:45	Dario Bercioux (I.4-online) Kazuhiko Kuroki (I.5) Nguyen Ba Phi (O.5) *(Chair: Nguyen Huy Viet)*	16:00 – 18:10	Nicola Colonna (I.8) Ding Pan (I.9) Thanh N. Pham (O.10) Bui Dinh Hoi (O.1) *(Chair:Nguyen Ngoc Linh)*		16:00 – 17:45	D. I. Kazakov (I.12-online) Nguyen Le Anh (O.15) Tran Viet Nhan Hao (O.16) Tran Chien Thang (O.17) *(Chair: Nguyen Quang Hung)*
	VTPS Meeting **(17:45)**			Gala dinner **(19:00)**		Closing

Conference Program

Tuesday, 30 July 2024

Opening Session
Chair: Tran Minh Tien

08:30 - 09:00	Registration
09:00 - 09:10	Opening
09:10 - 09:20	Announcement of 2024 VTPS Young Researcher Award
09:20 - 10:00	I.1 – Invited Excitonic physics and potential applications in two-dimensional materials **Vo Khuong Dien** (Division of Applied Physics, Dong Nai Technology University, Bien Hoa City, Vietnam)
10:00 - 10:10	Photo Session
10:10 - 10:30	Coffee break

Oral Session: *Condensed Matter Physics*
Chair: Bach Thanh Cong

10:30 - 11:10	I.13 – Invited Holographic Paradigm and Black Hole Thermodynamics **Bum-Hoon Lee** (Sogang University)
11:10 - 11:50	I.2 – Invited On the monotonicity of the renormalization group flow in nonequilibrium thermodynamics perspectives **Ki-Seok Kim** (Pohang University of Science and Technology)
11:50 - 12:15	O.2 – Oral Recent achievement of first-principles studies for applications in solar cell devices **Dang Minh Triet** (School of Education, Can Tho University, Viet Nam)
12:15 - 14:00	Lunch

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

14:00 - 14:40 I.3 – Invited
Linking the dark sector to the fermion mass hierarchy and the strong CP problem
Do Thi Huong (Institute of Physics, Vietnam Academy of Science and Technology)

14:40 - 15:05 O.3 – Oral
On the stability of de Sitter inflationary universes in some nontrivial extensions of the Starobinsky model
Do Quoc Tuan (PIAS, Phenikaa University)

15:05 - 15:30 O.4 – Oral
Flavor constraints on the BDW model
Tran Minh Hieu (Hanoi University of Science and Technology)

15:30 - 16:00 Coffee break

Oral Session: *Condensed Matter Physics*
Chair: Nguyen Huy Viet

16:00 - 16:40 I.4 – Invited
Exploring Chiral Spin States in Curved Spaces: Insights from Ring Geometries
Dario Bercioux (Donostia International Physics Center, Spain)

16:40 - 17:20 I.5 – Invited
Theoretical study on high T_c superconductivity in multilayer nickelates $La_3Ni_2O_7$ and $La_4Ni_3O_{10}$
Kuroki Kazuhiko (Osaka University)

17:20 - 17:45 O.5 – Oral
Transport and localization properties of excitations in the diluted Anderson model
Nguyen Ba Phi (Mientrung University of Civil Engineering)

17:45 - 18:30 VTPS Meeting

Wednesday, 31 July 2024

Poster Session 1
Chair: Trinh Xuan Hoang

08:30 - 10:00 P.1 – Poster
Electronic and optical properties of two dimensonal Bi2WO6 (010) structure: DFT study
Doan Thi Hien (Hanoi National University of Education)

08:30 - 10:00 P.2 – Poster

Transport coefficients of semiconductor bismuth oxytelluride

Đỗ Quỳnh Anh (Nanyang Technological University)

08:30 - 10:00 P.3 – Poster

The electron effective mass in the strong correlated quantum well wire electron fluid dependent finite-temperature

Lê Văn Tân (Van Lang University)

08:30 - 10:00 P.4 – Poster

The adsorption of CO2 on pentagonal SiC2 nanoribbon: A DFT study

Huynh My Linh (College of Natural Sciences - Can Tho University)

08:30 - 10:00 P.5 – Poster

Multielectron and multiorbital effects in in odd-even harmonic generation from CO molecules

Trần Thành (Ho Chi Minh City University of Education)

08:30 - 10:00 P.6 – Poster

Ultimate Precision of the Leptonic Mixing Angle θ_{23} and its Implications for the Leptonic Flavor Models

Phan To Quyen (IFIRSE, ICISE)

08:30 - 10:00 P.7 – Poster

Reaction rate of proton-deuteron radiative capture and its astrophysical implication

Do Huy Tho (Ho Chi Minh University of Education)

08:30 - 10:00 P.8 – Poster

Anharmonic EXAFS signals of Pb analyzed based on quantum anharmonic correlated Einstein model

Tong Sy Tien (University of Fire Prevention and Fighting)

08:30 - 10:00 P.9 – Poster

The astrophysical S-factor from proton-deuteron radiative capture within potential model

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

08:30 - 10:00 P.10 – Poster

Applying of complex scaling method to analyze the resonances in the weakly-bound nuclei

Trần Diệu Thùy (Đại học Sư phạm - Đại học Huế)

08:30 - 10:00 P.11 – Poster

Study of adsorption effects of acetone and acetonitrile on defected Penta-PdSe2 nanoribbons

Nguyễn Hải Đăng (Nam Can Tho University)

08:30 - 10:00 P.12 – Poster

Analyzing the relationship between population size and the dimension in the

problem of nuclear reactor fuel reload optimization using the SHADE method
Phan Thi Thuy Giang (Institute of Fundamental and Applied Sciences, Duy Tan University)

08:30 - 10:00 P.13 – Poster
Classification of the Mott transitions in multicomponent fermion systems
Trần Minh Tiến (Institute of Physics, VAST)

08:30 - 10:00 P.14 – Poster
The transfer of quantum entanglement in a rhombic 1/2 spins system
Le Duc Vinh (Tinh Gia 3 High school)

08:30 - 10:00 P.15 – Poster
Double exchange mechanism in topological insulators
Nguyen Hong-Son (Trade Union University)

08:30 - 10:00 P.16 – Poster
Multiphoton absorption process of an intense electromagnetic waves in monolayer graphene under the influence of both uniform electric and magnetic fields
Nguyen Dinh Nam (Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam)

08:30 - 10:00 P.17 – Poster
Solubility of Carbon Dioxide in Brine: A Molecular Simulation Study
Nguyen Tu Khai Nam (Duy Tan University)

08:30 - 10:00 P.18 – Poster
Investigation of Debye temperature and temperature-dependent EXAFS cumulants of Zn, Zr, α-Ti, Ru and Hf metals
Nguyen Thi Hong (Hong Duc university)

08:30 - 10:00 P.19 – Poster
Anisotropic exciton in two-dimensional black phosphorus in a uniform magnetic field
Lê Đỗ Đăng Khoa (Ho Chi Minh City University of Education)

08:30 - 10:00 P.20 – Poster
Missing energy method for searching heavy neutrinos via $B^- \to \ell^- N$ decays
Nguyen Hoang Duy Thanh (Institute of Physics, VAST)

08:30 - 10:00 P.21 – Poster
Metal-insulator phase diagram in the ionic Hubbard model with Coulomb disorder
Yen Thi Hai Nguyen (Institute of Physics)

08:30 - 10:00 P.22 – Poster
Dark charge: Probing neutrino mass and dark matter
Phung Van Dong (Phenikaa Institute for Advanced Study, Phenikaa University, Yen Nghia, Ha Dong, Hanoi, Vietnam)

08:30 - 10:00 P.23 – Poster

Magnetic and magneto-caloric investigation of amorphous systems in the description of disordered Ising model

Bach Giang (Faculty of Physics, VNU University of Science)

08:30 - 10:00 P.24 – Poster

A qualitative investigation of electrical conductivity in three-layer graphene structures

Le Thi Kieu Oanh (Department of Physics, University of Science- VNUHCM)

08:30 - 10:00 P.25 – Poster

The three-level optical Stark effect of exciton in GaAs disk-shaped quantum dots

Le Thi Dieu Hien (University of Sciences, Hue University)

08:30 - 10:00 P.26 – Poster

Excitonic systems in two-layer 2D parabolic quantum dots

Nguyen Hong Quang (Institute of Physics, VAST)

08:30 - 10:00 P.27 – Poster

Quantum simulation of collective neutrino oscillations

Vũ Văn Hướng (Hanoi National University of Education)

08:30 - 10:00 P.28 – Poster

Hydrodynamic simulation of the air flow and dust particle motion in a multistage impactor

Pham Tuan Kiet (Institute of physics, 10 Dao Tan)

08:30 - 10:00 P.29 – Poster

Thermal-Magnetic Effect on the Excited-State Energy Levels of a Plasma-Embedded Hydrogen Atom in a homogeneous Magnetic Field

Ly Duy-Nhat (HCMC University of Education)

08:30 - 10:00 P.30 – Poster

Low Energy Levels of Excitons in Monolayer TMDs in a Homogeneous Magnetic Field Using the FK Operator Method

Le Huu Duc (Ho Chi Minh City University of Education)

08:30 - 10:00 P.31 – Poster

Thermoelectric and magnetic properties of bismuth telluride with a Gd point defect

Tran Van Quang (Faculty of Electronics and Telecommunications VNU University of Engineering and Technology Vietnam National University, Hanoi)

08:30 - 10:00 P.32 – Poster

Investigating the damping states of drift velocity of electrons in GaAs semiconductor under the influence of external electric field

Thùy Thị Thu Lê (Duy Tan University, Da Nang)

08:30 - 10:00 P.33 – Poster
Questions of flavor physics and neutrino mass from a flipped hypercharge
N. T. Duy (Institute of Physics)

08:30 - 10:00 P.34 – Poster
Negative Poisson's ratio and anisotropic carrier mobility in ternary Janus Si_2XY (X/Y = S, Se, Te): First-principles prediction
Hieu Ngoc Nguyen (Duy Tan University)

08:30 - 10:00 S.1 – S Poster
Magnetic Bound State Using Neodymium Magnets
Do Hoang Minh (Hanoi Amsterdam High School for the Gifted)

08:30 - 10:00 S.2 – S Poster
The Dynamics of a Sphere Rolling Upwards on Diverging Inclined Guides
Hoang Pham Minh Khanh (Newton Grammar School)

10:00 - 10:30 Coffee break

Oral Session: *Molecular Physics, Quantum Optics and Quantum Information*
Chair: Hoang Ngoc Cam

10:30 - 11:10 I.6 – Invited
Highly accurate methods for molecular charge-transfer excited states
Tran Nguyen Lan (Vietnam National University, Ho Chi Minh City)

11:10 - 11:35 O.6 – Oral
Laser-target symmetry-breaking in high harmonic generation: from frequency shift to odd-even intensity modulation
Trieu Doan An (Computational Physics Key Laboratory, Department of Physics, Ho Chi Minh University of Education)

11:35 - 12:00 O.7 – Oral
Multielectron effects in High harmonic generation of HCN: Depending on laser pulse parameters
Hoàng Trọng Đại Dương (Ho Chi Minh City University of Education)

12:00 - 14:00 Lunch

Oral Session: *Particle, Nuclear and Astrophysics*
Chair: Tran Hoai Nam

14:00 - 14:40 I.7 – Invited
Imprint of pairing correlation in (n, γ) and Maxwellian-averaged cross sections of an odd-odd 166Ho nucleus
Nguyen Quang Hung (Institute of Fundamental and Applied Sciences, Duy Tan University)

14:40 - 15:05 O.8 – Oral
Joint polarizations of W pair production at the LHC: NLO EW corrections
Le Duc Ninh (Phenikaa university)

15:05 - 15:30 O.9 – Oral

Emergence of dark symmetry and neutrino mass scales from flavor symmetry.

Ranjeet Kumar (Department of Physics, Indian Institute of Science Education and Research - Bhopal, Bhopal Bypass Road, Bhauri, Bhopal 462066, India.)

15:30 - 16:00 Coffee break

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

16:00 - 16:40 I.8 – Invited

Koopmans-compliant functionals: a functional approach to spectroscopy

Colonna Nicola (Paul Scherrer Institut)

16:40 - 17:20 I.9 – Invited

First principles and machine learning studies of nanoconfined aqueous solutions in a large pressure-temperature range

Pan Ding (Hong Kong University of Science and Technology)

17:20 - 17:45 O.10 – Oral

Thermal stability of /$Sr_3Ti_2O_7$ catalyst under operando conditions revealed by machine learning enhanced global optimization

Pham Ngoc Thanh (Osaka University)

17:45 - 18:10 O.1 – Oral

Effects of a perpendicular electric field, electron-hole coupling, and dopants on the electronic phase transition in bilayer P6mmm borophene

Bui Dinh Hoi (Hue University of Education)

Thursday, 1 August 2024

08:00 - 16:00 Excursion

19:00 - 21:00 Gala dinner

Friday, 2 August 2024

Poster Session 2
Chair: Nguyen Hong Quang

08:30 - 10:00 P.35 – Poster

Distribution of the electric field inside an optical microcavity for different input angles

Le Tri Dat (Dong Nai Technology University)

08:30 - 10:00 P.36 – Poster

Systematic investigation on pairing phase transition in excited nuclei

Le Thi Quynh Huong (University of Khanh Hoa)

08:30 - 10:00 P.37 – Poster

Nonlinear oscillator model of experience-based decisions and application of normal distribution on Hanoi high school entrance exam grading

Chu Thuy Anh (Institut of Physics)

08:30 - 10:00 P.38 – Poster

Dynamical properties of photon-added squeezing-enhanced coherent state in the Jaynes-Cummings model

Le Thi Hong Thanh (Quang Nam University)

08:30 - 10:00 P.39 – Poster

Efficient qutrit gates in superconducting circuits using quantum optimal control

Tran Tuan Kha (Aalto University)

08:30 - 10:00 P.40 – Poster

A very low bandgap line-tunnel field effect transistor with channel-buried oxide and laterally doped pocket

Nguyễn Đăng Chiến (Dalat University)

08:30 - 10:00 P.41 – Poster

Nonlinear multi-photon Absorption of a Strong Electromagnetic Wave with electron-acoustic phonon scattering in infinite semi-parabolic Plus semi-inverse Squared Quantum Wells .

Dung Thi Bui (VNU University of Science)

08:30 - 10:00 P.42 – Poster

Quantum Computing with Cat qubits

Tran Thi Thanh Huyen (Hanoi National University of Education)

08:30 - 10:00 P.43 – Poster

Mass imbalance effects on microcavity exciton-polariton condensates

Nguyen Thi Hau (HaNoi University of mining and geology)

08:30 - 10:00 P.44 – Poster

Thermodynamic properties of monolayer honeycomb spin lattice

Nguyen Tu Niem (VNU University of Science)

08:30 - 10:00 P.45 – Poster

W Mass Anomaly and Physics Beyond the Standard Model

Đào Thị Nhung (Phenikaa University)

08:30 - 10:00 P.46 – Poster

Influence of cut-off frequency effect on resonance energy transfer and Casimir-Polder interaction

Nguyen Dung Chinh (IFAS, Duy Tan University)

08:30 - 10:00 P.47 – Poster

Magneto-optical absorption properties of monolayer transition metal dichalcogenides including electron-phonon interaction

Trần Ngọc Bích (Dong Thap University, Quang Binh University)

08:30 - 10:00 P.48 – Poster

First-principles prediction of the Ohmic contact and ultralow Schottky contacts in two-dimensional metal-semiconductor van der Waals heterostructures

Nguyễn Văn Chương (Học viện Kỹ thuật quân sự)

08:30 - 10:00 P.49 – Poster

Investigation of C and Si-doped 2D germanene quantum dots for potential nanotechnology applications

Hoang Van Ngoc (Thu Dau Mot University)

08:30 - 10:00 P.50 – Poster

Isospin mixing in the nuclear low-lying resonances

Le Tan Phuc (IFAS, Duy Tan University)

08:30 - 10:00 P.51 – Poster

Quantum Circuit Ansatz Structures for Ising Model & A Comparative Analysis of Classical and Quantum Optimization Methods

Le Duc Truyen (National Tsing Hua University)

08:30 - 10:00 P.52 – Poster

Study of nonlinear phenomena in advanced materials and devices: insights from distinct approaches

Tran Ky Vi (Faculty of Semiconductor Technology, Dai Nam University)

08:30 - 10:00 P.53 – Poster

Stability, electronic and mechanical properties of ZnO graphenylene-like nanosheet single and double layer: A first-principles study

Nguyễn Thị Thảo (Hong Duc University)

08:30 - 10:00 P.54 – Poster

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

Tran Thi Thanh Mai (Institute of Physics, VAST)

08:30 - 10:00 P.55 – Poster

Phenomenological Analogy between Gross-Pitaevskii Theory for Bose-Einstein Condensate mixtures in infinite space and Classical Mechanics

Pham Duy Thanh (Hanoi Pedagogical University 2)

08:30 - 10:00 P.56 – Poster

AI-Powered Mie Theory for Predicting Optical and Photothermal Heating of Nanoparticles

Ngô Thị Quế (Viện Nghiên cứu Tiên tiến Phenikaa, Trường Đại học Phenikaa)

08:30 - 10:00 P.57 – Poster

Machine Learning-Accelerated Design of Titanium Nitride Nanoring Metamaterial Absorbers for Broadband Solar Energy Harvesting

Đặng Bùi Nhật Lê (Khoa Khoa học và Kỹ thuật Vật liệu, Trường Đại học

Phenikaa, Hà Nội, Việt Nam)

08:30 - 10:00 P.58 – Poster

Investigating the conditions for CO2 sensing in the p-SiC2-SS nanoribbon model using DFT simulation method

Tran Yen Mi (Cantho University)

08:30 - 10:00 P.59 – Poster

Exploring Empirical Thermodynamic Quantities of Excited Nuclei Through Canonical Ensemble

Nguyen Ngoc Anh (Phenikaa Institute for Advance Study)

08:30 - 10:00 P.60 – Poster

Evaluation of Pafnucy deep neural network model for ligand based drug virtual screening

Nguyen Tien Cuong (University of Science, VNU)

08:30 - 10:00 P.61 – Poster

Investigating the site-dependent thermal stability of G6PD by coarse-grained and all-atom simulations

Nguyen Thi Thuy Nhung (Graduate University of Science and Technology)

08:30 - 10:00 P.62 – Poster

Vacuum stability using Vector like Quarks (VLQ)

Aman Verma (Department of Physics, University of Rajasthan, Jaipur, India)

08:30 - 10:00 P.63 – Poster

Investigation of phase transitions of the frustrated $J_1 - J_2$ Ising model on a square lattice in magnetic fields

Pham Huong Thao (Faculty of Physics, Hue University of Education)

08:30 - 10:00 P.64 – Poster

Neuropilin-1 protein may serve as a receptor for SARS-CoV-2 infection: Evidence from molecular dynamics simulations

Nguyen Hoang Linh (Institute of Fundemental & Applied Sciences, Duy Tan University)

08:30 - 10:00 P.65 – Poster

Influence of acoustic phonons on nonlinear optical-manegto absorption in special asymmetric hyperbolic quantum wells

Lê Đình (Hue University)

08:30 - 10:00 P.66 – Poster

Comparison of entanglement feature, EPR steering, and fidelity of quantum teleportation processes via pair coherent states by photon addition

Ho Sy Chuong (Dong Nai University)

08:30 - 10:00 P.67 – Poster

Mathematical model describes and analyzes the state of entity σ when entering the time domain P- The application creates new methods for storing and transmitting information data

Trần Đình An (Trường Đại học Sư phạm Kỹ thuật tp HCM)

08:30 - 10:00 P.68 – Poster

Investigation of the thermodynamic properties of ABO3 perovskite by the statistical moment method

Cao Huy Phuong (Faculty of Natural Sciences, Hung Vuong University)

08:30 - 10:00 P.69 – Poster

Effect of frequency detuning on absorption coefficient in a semiconductor quantum well with a three-levels ladder configuration

Tran Cong Phong (Trường Đại học Tôn Đức Thắng)

08:30 - 10:00 P.70 – Poster

Simulation of neutron and nuclear fragment productions in nucleus-nucleus interactions using the coupling UrQMD 3.4 + SMM model

Lê Thị Quỳnh Trang (Institute of Research and Development, Duy Tan University)

08:30 - 10:00 P.71 – Poster

Unrevealing the Roles of Defect Species in Absorption and Photo-degradation of Methylene Blue on the Nitrogen-Doped Anatase TiO2 Surface

Ngoc Linh Nguyen (Faculty of Material Sciences, Phenikaa university)

10:00 - 10:30 Coffee break

Oral Session: *Molecular Physics, Quantum Optics, and Quantum Information*
Chair: Le Dinh

10:30 - 11:10 I.10 – Invited

Regulated perturbation theory for two-dimensional atomic systems

Le Van Hoang (Ho Chi Minh City University of Education)

11:10 - 11:35 O.11 – Oral

Quantum computing with superconducting circuits

Nguyen Van Duy (Phenikaa University)

11:35 - 12:00 O.12 – Oral

Overview investigating the inverse Sauter effect in binary waveguide arrays

Trần Công Minh (Science and Technology Advanced Institute, Van Lang University)

12:00 - 14:00 Lunch

Oral Session: *Condensed Matter Physics*
Chair: Phan Van Nham

14:00 - 14:40 I.11 – Invited

Dielectric environment and Rydberg excitons in atomically thin semiconduc-

tors

Hoàng Ngọc Cầm (Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research)

14:40 - 15:05 O.13 – Oral

Photo-dressed state approach for generating unidirectional π-electron rotation in aromatic ring molecule

Hồ Quang Huy (computational physics laboratory K002, Ho Chi Minh city University of Education)

15:05 - 15:30 O.14 – Oral

Thermophysical Properties of Hydrogen in Brine

Hoang Hai (Institute of Fundamental and Applied Sciences, Duy Tan University)

15:30 - 16:00 Coffee break

Oral Session: *Particle, Nuclear and Astrophysics*
Chair: Nguyen Quang Hung

16:00 - 16:40 I.12 – Invited

Quantum corrections to cosmological potentials and the origin of the cosmological constant

D. I. Kazakov (Bogoliubov Laboratory of Theoretical Physics, JINR)

16:40 - 17:05 O.15 – Oral

Analysis of nuclear stability and deformation using spherical Skyrme HFBCS QRPA

Nguyen Le Anh (Department of Physics, Ho Chi Minh City University of Education)

17:05 - 17:30 O.16 – Oral

Odd-even mass differences of well and rigidly deformed nuclei in the rare earth region: A test of a newly proposed fit of pairing matrix elements

Tran Viet Nhan Hao (Hue University)

17:30 - 17:55 O.17 – Oral

Semileptonic decays $B_s \to D_s^{(*)}\tau\nu$ as probe for new physics

Tran Chien-Thang (Ho Chi Minh City University of Technology and Education)

17:55 - 18:15 Closing

Conference Abstracts

I.1 – Invited, VCTP-49

Excitonic physics and potential applications in two-dimensional materials

Vo Khuong Dien (1,2)

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Due to reduced dielectric screening and enhanced Coulomb interactions, two-dimensional (2D) materials exhibit strong excitonic effects, resulting in fascinating many-particle phenomena. In our current work, we discuss the remarkably versatile excitonic landscape, including bright excitons, spin-forbidden excitons, and momentum-forbidden dark excitons, by numerically solving the Bethe-Salpeter equation (BSE). We also explore potential applications, such as valleytronics and energy harvesting, highlighting the prominent role of excitonic effects. Keyworks: excitons in 2D Materials, BSE, Valleytronics, Förster-Induced Energy Transfer.

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Presenter: Vo Khuong Dien

I.2 – Invited, VCTP-49

On the monotonicity of the renormalization group flow in nonequilibrium thermodynamics perspectives

Kim Ki-Seok

Pohang University of Science and Technology

Following the entropy production description in nonequilibrium thermodynamics, we show the monotonicity of the renormalization group (RG) flow. In particular, we clarify the connection between the monotonicity of the RG flow (a- or c-theorem) and the entropy production (irreversibility). To investigate the monotonicity of the RG flow in the perspectives of nonequilibrium thermodynamics, we construct a holographic dual effective field theory of the cohomological type a la Witten, which manifests the RG flow in the level of an effective action. This effective field theory framework allows us to introduce various kinds of entropy functionals, where their

monotonic behaviors play a central role in the monotonicity of the RG flow. We discuss how the Gibbs-type entropy functional, the holographic entropy functional, the Perelman's entropy functional, and the Weyl anomaly are all deeply related, based on our holographic dual effective field theory.

Presenter: Ki-Seok Kim

I.3 – Invited, VCTP-49

Linking the dark sector to the fermion mass hierarchy and the strong CP problem

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We studied an extended two-Higgs-doublet model (2HDM) with a low-scale seesaw mechanism for neutrino mass generation. We propose a viable two-component dark matter candidate and provide a natural explanation for the observed fermion mass hierarchy. Here, only the third family acquires mass at the tree level, while the first and second families acquire mass via loop corrections mediated by the dark sector. The complex Cabibbo-Kobayashi-Maskawa (CKM) matrix arises at the one-loop level, and the strong CP phase, which is naturally suppressed, arises at the three-loop level. The decay channels that violate the lepton number and anomalous magnetic moments of muons are also studied.

Presenter: Do Thi Huong

I.4 – Invited, VCTP-49

Exploring Chiral Spin States in Curved Spaces: Insights from Ring Geometries

Dario Bercioux

Donostia International Physics Center, Spain

In this presentation, I will review the problem of electron spins moving in curved spaces, focusing on the problem of ring geometry. I will then demonstrate how chiral states in circular graphene pn junctions, subjected to normal magnetic fields and strong proximitized spin-orbit coupling, can imitate those of propagating spin carriers in semiconducting quantum rings. I will derive the effective one-dimensional Hamiltonian governing the zero modes' spin dynamics and calculate the geometric phase. I will also show that for a given polarity of the junction, a special point exists in parameter space where the spin is completely polarized along the radial direction in the graphene plane. Additionally, I will propose a novel quantum-Hall interferometer setup that can readily identify and observe these remarkable features. By employing this interferometer, I can gain valuable insights into the intricate nature of chiral spin states and their manifestation in ring geometries. Ref. D. Bercioux, D. Frustaglia & A. De Martino, Phys. Rev B 108, 225140 (2023) (on-line presentation)

Presenter: Dario Bercioux

I.5 – Invited, VCTP-49

Theoretical study on high T_c superconductivity in multilayer nickelates $La_3Ni_2O_7$ and $La_4Ni_3O_{10}$

Kazuhiko Kuroki

Department of Physics, Osaka University

Recent discovery of superconductivity with T_c exceeding 80K in a bilayer nickelate $La_3Ni_2O_7$ under pressure has sparked a renewed interest in the field of condensed matter physics. In fact, the possibility of superconductivity in this material was theoretically discussed in 2017 by the present author. There, the importance of the $d_{3z^2-r^2}$ orbital, which exhibits large interlayer hopping, being nearly half-filled was pointed out. In the present talk, we will revisit this problem and theoretically study a realistic model taking into account the lattice structure under pressure. By applying the fluctuation exchange method to the model, we investigate the possibility of spin fluctuation mediated superconductivity, and find a result consistent with T_c of 80K. Furthermore, we study the possibility of superconductivity in a trilayer nickelate $La_4Ni_3O_{10}$ in a similar manner. We find that the material can also exhibit superconductivity, which is confirmed by experiments.

Presenter: Kuroki Kazuhiko

I.6 – Invited, VCTP-49

Highly accurate methods for molecular charge-transfer excited states

Tran Nguyen Lan

Vietnam National University, Ho Chi Minh City

The chare transfer (CT) at the molecular level plays a fundamental role in many areas of chemistry, physics, biology and materials science. However, unlike conventional electronic states, CT is complicated to be accurately described because the character of CT states is different from ground states. Standard excited-state methods like linear response and perturbation theory are not sufficient to describe CT states. One needs to develop specific methods that can treat CT states equally to ground state. In this report, I will present our new methods to describe molecular CT states accurately. We will demonstrate the performance of our methods by studying intermolecular and intramolecular CT states.

Presenter: Tran Nguyen Lan

I.7 – Invited, VCTP-49

Imprint of pairing correlation in (n, γ) and Maxwellian-averaged cross sections of an odd-odd 166Ho nucleus

Le Tan Phuc (1), Tran Vu Dong (1), Nguyen Dinh Dang (2), Bui Minh Hue (3), Le Thi Quynh Huong (4), Balaram Dey (5), Nguyen Ngoc Anh (6), Nguyen Quang Hung (1)

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Dong, Hanoi, Vietnam

The present paper investigates the impact of pairing correlation on the nuclear level density (NLD) and radiative strength function (RSF) of an odd-odd and rare-earth 166Ho nucleus. By employing the exact thermal pairing (EP) solution in conjunction with both the temperature dependent independent-particle model (EP+IPM) for the NLD and the phonon damping model (EP+PDM) for the RSF, we achieve good agreement with the experimental NLD and RSF data, which have been recently extracted by using the Oslo method. Notably, without adding any extra parameters, our calculations successfully reproduce the pygmy dipole resonances (PDR) and a portion of the strength around the region of scissor resonance (SR) in the RSF. This suggests that the SR in this nucleus may be less pronounced than that obtained in the previous analysis within the phenomenological model. These features are the consequences of the EP and the couplings of the PDM phonon to all the particle-hole (ph), particle-particle (pp), and hole-hole (hh) configurations within the EP+PDM, thus insisting on the importance of the underlying physics involved in this model. Utilizing the obtained NLD and RSF, we predict the 165Ho(n,γ)166Ho and Maxwellian-averaged cross sections, which exhibit remarkable agreement with all the available experimental data from the Experimental Nuclear Reaction Data and Karlsruhe Astrophysical Database of Nucleosynthesis in Stars. These results reflect the imprint of the pairing correlation on those quantities [1].

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Presenter: Nguyen Quang Hung

I.8 – Invited, VCTP-49

Koopmans-compliant functionals: a functional approach to spectroscopy

Nicola Colonna

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Spectral properties are essential to understand or engineer materials: from photoemission spectra (widely used in recent years to characterize all possible topological properties) to transport (for ICT technologies) to light absorption (for energy harvesting) or emission (quantum technologies). To date, the most common electronic-structure approaches to reliably compute these quantities are based on Green's function theory. Despite the continuous improvement, these methods are still limited in system size and complexity due to their computational cost and complexity. As an alternative to Green's function methods, Koopmans spectral functionals provide a novel and functional approach to simultaneously and accurately describe ground state properties and charged excitations of atoms, molecules, nanostructures and periodic crystals. This is achieved by augmenting standard density functionals with simple but physically motivated orbital-density-dependent corrections that enforce the correct description of the charged excitation process. After introducing the general framework and its implementation, I will present numerical simulations showing the excellent agreement with experiments and state-of-the-art Green's function methods in predicting ionization potentials of a large set of molecules (the GW100 test set), photoemission and absorption spectra of organic donors and acceptors, band gaps and band structures of semiconducting and insulating crystalline materials. Finally, I will discuss the connection with Green's function theory arguing that the state-dependent Koopmans potentials act as a local

and orbital-dependent counterpart to the electronic self-energy, albeit including spin-dependent interactions and screening effects that are absent in standard diagrammatic approaches based on the random phase approximation (GW) and that would require the inclusion of self-screening and vertex corrections. Being this a functional framework, the straightforward advantages are that forces, and other derivatives are also readily accessible, and that the numerical parameters are those typical of density functional calculations.

Presenter: Colonna Nicola

I.9 – Invited, VCTP-49

First principles and machine learning studies of nanoconfined aqueous solutions in a large pressure-temperature range

Ding Pan

Department of Physics and Department of Chemistry, Hong Kong University of Science and Technology,

This talk presents a study on the impact of nanoconfinement on the physical and chemical properties of aqueous solutions, with a particular focus on the reactions of CO_2 in water under extreme pressure-temperature conditions. Carbon storage and transport below Earth's surface have significant implications for the carbon budget in the atmosphere, and underground aqueous solutions are often confined to the nanoscale. However, the molecular-scale chemical speciation and reaction mechanisms of these systems are not yet fully understood.

To address this issue, we performed extensive ab initio molecular dynamics (AIMD) simulations to investigate aqueous carbon solutions confined by graphene and stishovite (SiO_2) at 10 GPa and 1000 $\sim$ 1400 K. The results show that CO_2(aq) reacts more in nanoconfinement than in bulk. These findings suggest that CO_2(aq) in deep Earth is more active than previously thought, and confining CO_2 and water in nanopores may enhance the efficiency of mineral carbonation.

We further constructed Markov state models based on AIMD to elucidate the reaction mechanisms and kinetics of dissolved carbon in supercritical water both in the bulk and nanoconfined states. Unlike many previous molecular simulations using enhanced sampling methods, our method can automatically identify complex reaction coordinates and pathways with multiple intermediates using unsupervised machine learning techniques instead of a priori human speculation. In the bulk solution, CO_2 tends to directly react with H_2O or OH^- to generate HCO_3^- and H_2CO_3(aq), whereas under graphene nanoconfinement the dissolution of CO_2 involves the pyrocarbonate ($C_2O_5^{2-}$(aq)) ion as an intermediate state. While it is known that pyrocarbonate does not exist in aqueous solutions, our study suggests that the extreme hydrophobic confinement may greatly enhance the stability of pyrocarbonate ions in water. Our study provides valuable insights into the reaction kinetic network of aqueous carbon, yielding significant implications for the deep carbon cycle and the sequestration of CO_2. Combining quantum molecular dynamics with Markov state models shows great potential to elucidate complex reaction pathways and kinetics.

References:

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Presenter: Pan Ding

I.10 – Invited, VCTP-49

Regulated perturbation theory for two-dimensional atomic systems

Le Van Hoang

HCMC University of Education

We have developed a novel approach called regulated perturbation theory for solving the Schrodinger equation of a two-dimensional hydrogen atom in an external field by combining the conventional perturbation method with several elements of the Feranchuk-Komarov method. This includes the Levi-Civita transformation, the algebraic calculation technique using the annihilation and creation operators, and the introduction of a free parameter to optimize the convergence rate of the perturbation series. The application is demonstrated for excitons in monolayer transition-metal dichalcogenides in a magnetic field.

Presenter: Le Van Hoang

I.11 – Invited, VCTP-49

Dielectric environment and Rydberg excitons in atomically thin semiconductors

Hoang Ngoc Cam

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The dielectric environment contributes to electrostatic interaction in atomically thin (2D) semiconductors, rendering their excitons environmentally sensitive. Extended Rydberg excitons, compatible with modern semiconductor technologies and thus offering prospects for quantum simulation, quantum optics and quantum sensing, have been observed in a 2D semiconductor up to n=11. How the environment affects 2D Rydberg excitons is still poorly understood. Here we exploit a variational approach for modeling 2D Rydberg excitons within an effective mass approximation. We formulate Rydberg exciton binding energies and wave functions in their systematic relation to the dielectric contrast of the 2D semiconductor and its immediate surroundings. The model demonstrates the environmental role in determining both the overall picture of the Rydberg exciton spectrum and individual features of each. Furthermore, it provides a scaling rule for Rydberg excitons in moderate and high screening media that resembles the behavior of their conventional 2D counterparts, but is governed by a function of dielectric contrast. Available experimental observations support our model, which clarifies fundamental Rydberg exciton physics in 2D semiconductors and can be used for dielectric control of Rydberg exciton features through dielectric engineering.

Presenter: Hoàng Ngọc Cầm

I.12 – Invited, VCTP-49

Quantum corrections to cosmological potentials and the origin of the cosmological constant

D. I. Kazakov

Bogoliubov Laboratory of Theoretical Physics, JINR, Dubna, Russia

We demonstrate how one can calculate the leading quantum corrections to arbitrary scalar

potentials even in non-renormalizable theories. We derive the generalised RG equation for the effective potential which takes into account all the leading terms in all orders of perturbation theory, just like it takes place in renormalizable case. Application of this formalism to the co-called alpha-attractors in inflationary cosmology leads to increase of the potential at the minimum which can be interpreted as appearance of the cosmological constant due to quantum corrections. Choosing the set of parameters dictated by inflation scenario one can get the value of the cosmological constant satisfying the modern data.

Presenter: D. I. Kazakov

I.13 – Invited, VCTP-49

Holographic Paradigm and Black Hole Thermodynamics

Bum-Hoon Lee

Sogang University, Seoul, Korea

The holography principle says that the quantum field theories in the d-dimensional spacetime can equivalently be described by the one-dimension higher d+1 dimension classical gravity system with the negative cosmological space-time (so-called anti-de Sitter (AdS) space). For example, the coupling constant in the quantum field theory is related to the "size" of the AdS space. This provides a new paradigm to describe the strongly interacting quantum system, such as nuclear interaction or strongly correlated system, in terms of a corresponding classical gravity system. The black hole, a long-time studied object, is known to have thermal properties with the so-called Hawking temperature. Hence, the finite temperature quantum system will be related to the gravity theory with the black hole. The crucial step in relying on this new paradigm is finding the right gravity system. In this presentation, we will explain the underlying key ideas and concepts of the holographic principle and the black hole thermodynamics with some examples.

Presenter: Bum-Hoon Lee

O.1 – Oral, VCTP-49

Effects of a perpendicular electric field, electron-hole coupling, and dopants on the electronic phase transition in bilayer P6mmm borophene

Le Thi Thu Phuong (1), Nguyen Ngoc Hieu (2), Huynh Vinh Phuc (3), Vo Thi Tuyet Vi (4), Bui Dinh Hoi (1)

(1) University of Education, Hue University; (2) Duy Tan University; (3) Dong Thap University; (4) University of Medicine and Pharmacy, Hue University

We investigate the influence of external stimuli, including a perpendicular electric field, electron-hole coupling between sublayers (excitonic effects), and dopants on the potential electronic phase transitions in bilayer P6mmm borophene. Our focus is on key electronic properties such as the band structure and density of states. Our findings reveal that the pristine lattice is metal with Dirac cones around the Fermi level, where their intersection forms a nodal line. The system undergoes transitions to a semiconducting state – elimination of nodal line – with a perpendicular electric field and a semimetallic state – transition from two Dirac cones to a single Dirac cone – with combined electric field and excitonic effects. Notably, with these, the system retains its massless Dirac-like bands characteristic at finite energy. However, introducing a dopant still leads to a metallic phase, but the Dirac-like bands become massive. Considering all these effects, the

system ultimately reaches a semiconducting phase with massive Dirac-like bands. These results hold significance for optoelectronic applications.

Presenter: Bui Dinh Hoi

O.2 – Oral, VCTP-49

Recent achievement of first-principles studies for applications in solar cell devices

Dang Minh Triet

School of Education, Can Tho University, Viet Nam

Urgent global energy demand and the climate crisis lead to a global drive of seeking renewable and sustainable energy sources such as solar energy to reduce the cost of generating electricity and endure energy security. However, due to the limited commercial light-to-energy conversion efficiency of current conventional solar cell materials, the need of developing advanced nanostructured materials to enhance the efficiency of solar absorbers to exceed the Shockley-Queisser limit is crucial for the next-generation solar cell devices. Two-dimensional (2D) materials such as silicene, boron nitride, molybdenum disulfide (MoS2), phosphorene, and transition metal dichalcogenides (TMDs) with unique electronic, optical, and spintronic properties received enormous attention in the semiconductor industry. Among this class of materials, blue phosphorene, cadmium selenide (CdSe), rhenium dichalcogenides (ReS2) and their related morphological configurations with tunable band gaps and highly mobile charge carriers are considered as potential candidates for applications in photovoltaic devices. Here, using first-principles calculations with some available experimental observations, I would like to review our group's recent interesting achievements of optical and transport properties upon introducing different types of vacancies or structural modification to the hosted materials. We employ the generalized gradient approximation with the Perdew-Burke-Ernzerhof (PBE) and the hybrid density functional theory model functionals such B3LYP, HSE06, M06-2X as exchange-correlation functionals with or without van der Waals approximations to compute the equilibrium structure, vibration spectra and optoelectronic properties of several TMD materials. We also evaluate the impact of vacancies and material deformations on device performance using the non-equilibrium Green function formalism with density functional based tight-binding methods. The polaronic or excitonic states formed by these investigated materials, on the one hand, induce more new absorption frequencies in the visible light range; on the other hand, they reduce or increase the current passing through these scattering regions depending on their morphology. Our results highlight the sensitivity of the chosen materials in applications for solar cell devices.

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Presenter: Dang Minh Triet

O.3 – Oral, VCTP-49

On the stability of de Sitter inflationary universes in some nontrivial extensions of the Starobinsky model

Tuan Q. Do

Phenikaa Institute for Advanced Study, Phenikaa University

We will present main results of our recent investigations in the stability of de Sitter inflationary universes in some nontrivial extensions of the Starobinsky model. Our results could be useful for determining whether these extensions are suitable for either an inflationary phase of the very early universe or an accelerated expansion phase of the late time universe.

Presenter: Do Quoc Tuan

O.4 – Oral, VCTP-49

Flavor constraints on the BDW model

Tran Minh Hieu (1), Dinh Quang Sang (2)

(1) Hanoi University of Science and Technology; (2) VNU University of Science, Vietnam National University - Hanoi

In the BDW model, a $U(1)_X$ sector consists of vectorlike fermions and scalars is introduced beside the standard model particle content. We have investigated various flavor physics constraints on this model including the B-meson decays, CKM unitarity, and the muon $g-2$. The viable parameter regions are identified.

Presenter: Tran Minh Hieu

O.5 – Oral, VCTP-49

Transport and localization properties of excitations in the diluted Anderson model

Ba Phi Nguyen (1,2) and Kihong Kim (3)

(1) Department of Basic Sciences, Mientrung University of Civil Engineering, Tuy Hoa 620000, Vietnam; (2) Mathematics and Physics Research Group, Mientrung University of Civil Engineering, Tuy Hoa 620000, Vietnam; (3) Department of Physics, Ajou University, Suwon 16499, Korea

We present a numerical study of the transport and localization properties of excitations in one-dimensional lattices with diagonal disordered mosaic modulations, which are characterized by the integer-valued modulation period κ the disorder strength W. For different values of κ and W, we perform extensive numerical calculations of the disorder-averaged physical quantities. We find that while the conventional Anderson localization behavior takes place for most values of energy, there is a discrete value set of energies (the so-called quasiresonance energy) at which show a power-law localization behavior. When the wave packet's initial momentum satisfies the

quasiresonance condition, we observe a subdiffusive spreading of the wave packet.

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Presenter: Nguyen Ba Phi

O.6 – Oral, VCTP-49

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

Doan-An Trieu, Van-Hoang Le, Ngoc-Loan Phan

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Although the 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 phenomena. In this report, we provide a comprehensive picture of these two nonlinear optical phenomena, unifying them through a common origin - asymmetry of the laser-target system. By tuning asymmetric laser-target systems, we discover a transition from the harmonic frequency shift to the odd-even intensity modulation upon increasing the duration of the driving laser pulse. Specifically, these phenomena are observed simultaneously for laser pulses with intermediate pulse duration. For numerical evidence, we solve the time-dependent Schrödinger equation, while insight into the underlying physics is obtained from a simplified analytically tractable model. Understanding the asymmetric characteristics reflected in the HHG as provided is crucial for retrieving laser-target information, sampling external fields, and probing molecular dynamics.

Presenter: Trieu Doan An

O.7 – Oral, VCTP-49

Multielectron effects in High harmonic generation of HCN: Depending on laser pulse parameters

Duong D. Hoang-Trong (1), Ngoc-Loan Phan (1), Doan-An Trieu (1), and Van-Hoang Le (1)

(1) Ho Chi Minh City University of Education, 280 An Duong Vuong Street, Ward 4, District 5, Ho Chi Minh City 72711, Vietnam

In recent decades, the progress of laser technologies has resulted in the discovery of various nonlinear effects [1-4]. These nonlinear effects, such as above-threshold ionization (ATI), high-energy ATI (HATI), nonsequential double ionization (NSDI), and high-order harmonic generation (HHG) [1-4], have potential to imply extracting time-resolved imaging and investigating dynamics within atoms and molecules [5, 6]. As a result, a deep physics understanding and accurate theoretical explanations of these nonlinear effects that are consistent with experimental observations are required. Solving time-dependent Schrödinger equation (TDSE) using the single active electron (SAE) model which is a low-cost method is a common way for investigating these phenomena theoretically [7-9]. Previous works ansatz highest occupied molecule orbital (HOMO) dominantly contributes to highly nonlinear spectra, such as HHG, compared to lower-lying orbitals [10-12]. However, subsequent studies have revealed the imprint of lower-lying orbitals. The coupling between HOMO and lower-lying orbitals leads to electron-electron interactions between

MOs, called the multielectron effect. This effect offers to extract electron-electron dynamics on attosecond time scales, a significant topic in Strong-field Physics.

To determine the contribution of each MO, an advanced approach such as time-dependent density-functional theory (TDDFT) is applied [13-15]. However, due to the new target, HCN molecules, there is disagreement in these researches about the contribution of HOMO and HOMO-1 [13, 15]. Furthermore, these simulations did not consider the permanent dipoles of each MO, which is required for dissymmetrical molecules like HCN.

In this work, we discerned the contribution of HOMO and HOMO-1 in HHG spectra of HCN by solving the TDSE with SAE approximation that mimics the energies and permanent dipoles of both HOMO and HOMO-1. We explored the imprint of multielectron and the competition in contributing to HHG spectra of HOMO and HOMO-1 depending on the laser parameters. This explained the disagreement in previous studies [13, 14].

References:

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Presenter: Hoàng Trọng Đại Dương

O.8 – Oral, VCTP-49

Joint polarizations of W pair production at the LHC: NLO EW corrections

Thi Nhung Dao, Duc Ninh Le

Phenikaa University, Hanoi

In this talk, we present new results of next-to-leading order electroweak corrections to the doubly

polarized W+W- production cross sections at the LHC, via the full leptonic final state. This calculation has been recently achieved independently by two groups: one in Germany and our group in Vietnam. A comparison of the two results will be presented.

Presenter: Le Duc Ninh

O.9 – Oral, VCTP-49

Emergence of dark symmetry and neutrino mass scales from flavor symmetry.

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We worked on a model for hybrid neutrino mass generation, wherein scotogenic dark sector particles, including dark matter, are charged non-trivially under the A_4 flavor symmetry. The spontaneous breaking of the A_4 group to the residual Z_2 subgroup results in the "cutting" of the radiative loop. As a consequence the neutrinos acquire mass through the hybrid "scoto-seesaw" mass mechanism, with the residual Z_2 subgroup ensuring the stability of the dark matter. The flavor symmetry also leads to several predictions including the normal ordering of neutrino masses and "generalized $\mu - \tau$ reflection symmetry" in leptonic mixing. Additionally, it gives testable predictions for neutrinoless double beta decay and a lower limit on the lightest neutrino mass. Finally, the model allows only scalar dark matter, whose mass has a theoretical upper limit of ~ 600 GeV, with viable parameter space satisfying all dark matter constraints, available only up to about 80 GeV. Various aspects of this highly predictive framework can be tested in both current and upcoming neutrino and dark matter experiments.

Presenter: Ranjeet Kumar

O.10 – Oral, VCTP-49

Thermal stability of /$Sr_3Ti_2O_7$ catalyst under operando conditions revealed by machine learning enhanced global optimization

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Self-regenerative materials are pivotal for developing thermally-stable catalysts. Perovskite-supported metal nanoparticles (NPs) have shown promise. However, our understanding of the stability of perovskite-supported metal NPs remains limited. Herein, we elucidate the thermal stability of $Pd/Sr_3Ti_2O_7$ (STO-327) [1] by operando computer simulation that combines density functional theory (DFT) with machine learning-enhanced global optimization (GOFEE) [2] and thermodynamics [3]. First, we first elucidate the stability of Pd/STO-327 against the Pd dissolution deactivation by considering the thermodynamic phase diagram of Pd-doped STO-327. Second, we apply the GOFEE method based on an evolutionary algorithm and a Gaussian process regression, which is trained on the fly with DFT calculations, to the search for the stable structures of Pd_xO_y on STO-327. We find that the formation of PdO-like clusters enhances their binding strength to the support, inhibiting the agglomeration (sintering) of the Pd_xO_y NPs. By comparing with γ-Al_2O_3 supported Pd clusters, the interactions between Pd clusters and STO-327 surfaces are much stronger due to strong charge transfer interaction, highlighting that the

Pd/STO-327 catalysts have a higher thermal stability. This work may provide a guideline for the rational design of the thermally stable catalyst against sintering.

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Presenter: Pham Ngoc Thanh

O.11 – Oral, VCTP-49

Quantum computing with superconducting circuits

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Superconducting circuits have emerged as a leading platform for quantum computing, offering scalable and highly coherent qubits. This presentation covers the design and operation of superconducting qubits, recent advancements in coherence and gate fidelity, and the future challenges in the field.

Presenter: Nguyen Van Duy

O.12 – Oral, VCTP-49

Overview investigating the inverse Sauter 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 decaying 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 inverse Sauter effect by launching a Dirac soliton in binary waveguide arrays where the smooth transition region of the inverse potential step can be easily realized if we modify the effective refractive indices of the waveguides so that the smooth declining transition region of the inverse potential step can be described by a linear, exponential, or sinusoidal function [8]. As expected, if the transition obeys the linear and sinusoidal laws, then the inverse Klein tunneling is practically suppressed if the transition width is comparable to or larger than the Compton length. In this talk, we demonstrate that the analytical transmission coefficient in the discrete model with BWAs is in strikingly perfect agreement with the simulations-based results.

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Presenter: Trần Công Minh

O.13 – Oral, VCTP-49

Photo-dressed state approach for generating unidirectional π-electron rotation in aromatic ring molecule

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The laser driven π-electron rotation in aromatic ring molecules is one of the typical topics of photo-controlled charged migration, which has contributed to a development of the next-generation organic electronics devices. Recently much attentions have been concentrated on the generation of unidirectional rotation of π-electron, which is induced by a strong electric field. The rapidity of unidirectional rotation has been estimated by the orbital angular momentum of π-electron using quantum chemical calculations. The unidirectional angular momentum has been investigated by irradiating the high-symmetry aromatic molecule with the UV circularly polarized laser pulse (CP laser) to instantly populate from the ground state to the pair of degenerate electronic states, which forms the angular momentum state [1]. Although low-symmetry group do not contain the pair of degenerate states, the mechanism of dressed states has been introduced utilizing the pair of equal frequency continuous linearly polarized lasers to generate the stationary angular momentum [2]. Here, the pair of linearly polarized lasers with distinct polarization directions is combined to form an elliptically polarized laser (EP laser). However, treatment of π-electron rotation of dressed states in the aromatic ring molecules has not been discussed in a fully satisfactory way in preceding works. In our research, the dressed state approach has been used to solve the time-dependent Schrödinger equation in the aromatic molecule with any fold symmetry (high and low symmetry) in CP or EP laser (more generally, helical laser) in quasi-quantum mechanics. In the three electronic states model, including ground and pair of degenerate excited states in case of high symmetry or pair of quasi-degenerate excited states in case of low symmetry, three dressed states have been generated, each can generate angular momentum, in which the signal of each angular momentum is associated with the corresponding dressed state. One of three angular momentums represents a 'counter-intuitive' of π-electron

rotation in the aromatic ring, indicating that the electron's direction rotation is opposing the direction rotation of electronic field, this cannot be explained using classical mechanics and has been considered as quantum behavior. The angular momenta of the rest two dressed states, the direction of π-electron rotation is same as that of the electronic field, which can be understood using classical mechanics, therefore two dressed states indicate the 'intuitive' rotation of π-electron. [1] I. Barth, J. Manz, Y. Shigeta and K. Yagi, "Unidirectional Electronic Ring Current Driven by a Few Cycle Circularly Polarized Laser Pulse: Quantum Model Simulations for Mg-Porphyrin," J. Am. Chem. Soc, vol. 128, no. 21, pp. 7043-7049, 2006. [2] M. Yamaki, Y. Teranishi, H. Nakamura, S. H. Lina and Y. Fujimura, " The generation of stationary π-electron rotations in chiral aromatic ring molecules possessing non-degenerate excited states," Phys. Chem. Chem. Phys, vol. 18, no. 3, pp. 1570-1577, 2016.

Presenter: Hồ Quang Huy

O.14 – Oral, VCTP-49

Thermophysical Properties of Hydrogen in Brine

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Hydrogen is considered a viable solution for storing surplus renewable energy through electrolysis [1]. This leads to a requirement for efficient hydrogen storage solutions. Deep saline aquifers, which offer vast storage capacity and widespread distribution, are promising options for such storage [2]. The optimization of such storage systems requires accurate knowledge of hydrogen's thermophysical properties such as solubility, diffusivity, surface tension ... in these conditions [2]. However, obtaining experimental data on these properties is challenging or insufficient due to the complexity and the extreme conditions of underground geological formations. Molecular simulations have emerged as effective alternatives to experiments in dealing with such situations [3]. This presentation will introduce advanced simulation methods including Monte-Carlo and Molecular Dynamics [3], and present some simulation results on the solubility and diffusivity of H2 in NaCl brine at high pressures and high temperatures [4-5]. In particular, physical interpretations on the results will also be discussed [4-5]. In addition, some correlations based on the simulation results have been developed to predict the solubility and diffusivity of H2 in brine.

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Presenter: Hoang Hai

O.15 – Oral, VCTP-49

Analysis of nuclear stability and deformation using spherical Skyrme HFBCS QRPA

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The spherical Hartree-Fock (HF) Bardeen-Cooper-Schrieffer (BCS) quasiparticle random-phase approximation (QRPA) using Skyrme forces can explore the stability and softness of nuclei against quadrupole, octupole [1], and hexadecapole deformations [2]. Within the spherical self-consistent mean-field framework, the ground-state deformation of even-even nuclei can be identified when the HFBCS-QRPA stability matrix is not positive-definite [3]. Conversely, if the RPA stability matrix is positive-definite, static polarizability can serve as an indicator of stiffness. This method offers a computationally light and theoretically sound approach to identify potential softness or deformation in nuclei. By highlighting the influence of the shell-driving mechanism, our research provides insights into the evolutionary aspects of nuclear deformation. Acknowledgment: This work was funded by the Master, PhD Scholarship Programme of Vingroup Innovation Foundation (VINIF), code VINIF.2023.TS.003.

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Presenter: Nguyen Le Anh

O.16 – Oral, VCTP-49

Odd-even mass differences of well and rigidly deformed nuclei in the rare earth region: A test of a newly proposed fit of pairing matrix elements

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We discuss a test of a recently proposed approach to determine average pairing matrix elements within a given interval of sp states around the Fermi level λ as obtained in the so-called uniform gap method (UGM). It takes stock of the crucial role played by the averaged single particle (sp) level density $\sim \rho(e)$. These matrix elements are deduced within the UGM approach, from microscopically calculated $\sim \rho(e)$ and gaps obtained from analytical formulae of a semi-classical nature. Two effects generally ignored in similar fits have been taken care of. They are: a) the correction for a systematic bias in choosing to fit pairing gaps corresponding to equilibrium deformation solutions as discussed by Moller and Nix [Nucl. Phys. A 476, 1 (1992)] and b) the correction for a systematic spurious enhancement of $\rho(e)$ for protons in the vicinity of λ, due to the use of the local Slater approximation for the treatment of the Coulomb exchange terms in most calculations (see e.g. [Phys. Rev C 84, 014310 (2011)]). This approach has been deemed to be very efficient upon performing Hartree-Fock + BCS (with seniority force and self-consistent blocking when dealing with odd nuclei) calculations of a large sample of well and rigidly deformed even-even rare-earth nuclei. The reproduction of their experimental moments of inertia has been found to be at least of the same quality as what has been obtained in a direct fit of these data [Phys. Rev C 99, 064306 (2019)]. We extend here the test of our approach to the reproduction, in the same region, of three point odd-even mass differences centered on odd-N or odd-Z nuclei. The agreement with the data is again roughly of the same quality as what has been obtained in a direct fit, as performed in the above reference.

Presenter: Tran Viet Nhan Hao

O.17 – Oral, VCTP-49

Semileptonic decays $B_s \to D_s^{(*)}\tau\nu$ as probe for new physics

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We study the semileptonic decays $B_s \to D_s^{(*)}\tau\nu$ as a promising probe for new physics (NP) beyond the standard model (SM). The extension of the SM is done through the introduction of four-fermion operators beyond the $V - A$ structure with the corresponding Wilson coefficients characterizing their contribution. The constraints on these coefficients are obtained from recent experimental data. Form factors describing hadron transitions are calculated in our covariant quark model with infrared confinement. Theoretical predictions for the full set of observables in these chanels are provided. We compare our results with other studies and analyze possible NP effects to be tested in future experiments.

Presenter: Tran Chien-Thang

P.1 – Poster, VCTP-49

Electronic and optical properties of two dimensonal Bi2WO6 (010) structure: DFT study

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Bi2WO6 is recognized as a promising material for CO2 reduction due to its distinctive sand-

wich structure, suitable energy band configuration, and excellent thermal and photostability. Its crystal structure comprises alternating [Bi2O2]2+ and [WO4]2– ionic layers along the [010] direction, with significant hybridization between O 2p and Bi 6s orbitals in the [Bi2O2]2+ layer, providing numerous reactive sites that enhance its photoactivity. In this study, we employ density functional theory (DFT) calculations to investigate the electronic and optical properties of the two-dimensional Bi2WO6 (010) structure. The partial density of states reveals that the O 2s and O 2p orbitals contribute predominantly to the energies below the Fermi level, while the W 5d and Bi 6p orbitals are the primary contributors above the Fermi level. By analyzing the complex dielectric function, we compute various optical parameters, including the refractive index, extinction coefficient, reflectivity, and absorption coefficient, to further elucidate the optical properties of Bi2WO6 (010). The static dielectric constant is found to be 179, and the static refractive index is 13.6. This study provides insights that could further enhance the photocatalytic performance of Bi2WO6 (010).

Presenter: Doan Thi Hien

P.2 – Poster, VCTP-49

Transport coefficients of semiconductor bismuth oxytelluride

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Semiconductor bismuth telluride is emerging as a promising candidate for thermoelectric applications due to its impressively low lattice thermal conductivity. In this study, we present the results of calculations on the transport coefficients of this material. We discuss the relationship between electronic ground states and transport properties, characterized by the Seebeck coefficient, electrical conductivity, electronic thermal conductivity, and power factor. Our analysis yields compelling results demonstrating the dependence of transport properties on doping levels and temperature. This discovery highlights a significant challenge in improving the thermoelectric figure of merit at elevated temperatures.

Presenter: Đỗ Quỳnh Anh

P.3 – Poster, VCTP-49

The electron effective mass in the strong correlated quantum well wire electron fluid dependent finite-temperature

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We calculate the finite-temperature thermal effective mass for one-dimensional systems within the plasmon-pole approximation. We find that the calculated temperature denpendent effective mass including exchange and correlation is non-monotonic. In quantum wire systems at low-density the mass effective decreases as first with increasing the density, but after reaching a minimum it increases as the density is raised further. We find the leading order temperature correction to the mass effective within the plasmon-pole approximation to be increase at low temperature for all the densisty.

Presenter: Lê Văn Tân

P.4 – Poster, VCTP-49

The adsorption of CO2 on pentagonal SiC2 nanoribbon: A DFT study

Huynh My Linh, Tran Yen Mi, Huynh Anh Huy, Nguyen Thi Anh Thu

Can Tho University

Based on DFT simulation method, it is could say that there is a possibility of chemical bonding between CO2 and p-SiC2-SS substrate. However, because CO2 is a non-polar molecule, the choice of initial configuration between them plays an important role for building this kind of bonding. In addition, our results also show that increasing the CO2 concentration does not significantly change the interaction between them. This research will serve as a basis for studying the sensing ability of p-SiC2-SS for CO2 molecule.

Presenter: Huynh My Linh P.5 – Poster, VCTP-49

Multielectron and multiorbital effects in in odd-even harmonic generation from CO molecules

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Implementing intense laser with an ultra-short pulse duration deepens our understanding of laser-molecule interactions and nonlinear effects. Among the non-linear effects, high-order harmonic generation (HHG) has become a powerful tool in extracting molecules' structures [1], probing molecular dynamics [2,3], and producing attosecond pulse trains or isolated attosecond pulse [4,5]. For a long time, it is popularly acceptable that the highest occupied molecular orbital (HOMO) dominantly contributes to HHG compared to lower-lying orbitals [6,7]. As a result, the single-active electron (SAE) model is usually applied to simulate the HHG emitted from atoms molecules [7,8]. However, recently, it is shown that multielectron effect impacts the HHG spectra of specific atoms and molecules [9,10]. We also demonstrated that multielectron effect described via dynamic core-electron polarization (DCeP) strongly affect the odd-even HHG from CO molecule [11,12]. Moreover, only even-to-odd ratio is reduced by one order of magnitude, making it agrees with experimental data [13,14]. However, since DCeP is the coupling of the laser-induced polarization of the core electron with the active electron, it is the average effect of the core electron. It is still desirable to identify which lower-lying orbitals contribute to odd-even HHG spectra from CO molecule? In this work, we study the multielectron and multiorbital effects on the HHG of CO. The HHG spectrum is calculated using time-dependent density functional theory (TDDFT) embedded in OCTOPUS source code. The obtained spectra are validated by those solving the time dependent Schrödinger equation considering DCeP effect. The results show that the lower-lying orbitals strongly contribute into HHG spectra. More specifically, when the angles between the laser electric polarization and molecular axis (called orientation angle) are larger than 600, both HOMO and HOMO-1 contribute in HHG. In particular, HOMO dominates in low-order HHG while HOMO-1 governs HHG orders after cutoff. More interesting, we find out that for harmonics just before and at cutoff, HOMO contribute to odd harmonic while HOMO-1 to even ones. The time-frequency analysis is proceeded to explain

the observed results.

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Presenter: Trần Thành

P.6 – Poster, VCTP-49

Ultimate Precision of the Leptonic Mixing Angle θ_{23} and its Implications for the Leptonic Flavor Models

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Neutrino oscillation, a quantum mechanics phenomenon where one type of neutrino flavor can invert into others when traveling, revealing that neutrinos have mass and that leptons mix, surpasses the explanatory scope of the Standard Model. In the weak interaction basis, neutrino flavor eigenstates $(\nu_e, \nu_\mu, \nu_\tau)$ are related to neutrino mass eigenstates (ν_1, ν_2, ν_3) through the unitary leptonic mixing matrix U_{PMNS}, parameterized by three mixing angles $(\theta_{12}, \theta_{13}, \theta_{23})$ and one CP-violation phase (δ_{CP}), with the precision measurement of U_{PMNS} being one of primary objectives of current and future neutrino experiments. Among the three leptonic mixing angles, the θ_{23} angle, which characterizes the fractional contribution of the two flavor eigenstates ν_μ and ν_τ in the mass eigenstate ν_3, is known to be the largest (close to $\pi/4$) but the least precisely measured. Up-to-date data from neutrino oscillation experiments neither exclude the maximal mixing $\theta_{23} = \pi/4$ hypothesis nor determine distinctly its octant preference. This work revisits the ambiguity in the measurement of this angle in conjunction with other leptonic mixing parameters and investigates its ultimate precision measurement with two upcoming gigantic accelerator-based long-baseline neutrino experiments, Hyper-Kamiokande and DUNE, as well as joint possible future neutrino facilities like ESSnuSB and Neutrino Factory. The implication of this precise measurement of the mixing angle θ_{23} in examining the leptonic flavor models is also discussed.

Presenter: Phan To Quyen

P.7 – Poster, VCTP-49

Reaction rate of proton-deuteron radiative capture and its astrophysical implication

Do Huy Tho (1), Nguyen Le Anh (1), Dao Nhut Anh (1), Nguyen Huu Nha (2)

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We investigate the reaction rate of proton-deuteron (pd) radiative capture based on our calculated astrophysical S factor [1,2]. Using the potential model framework, we compute the astrophysical S factors and reaction rates for both $E1$ and $M1$ transitions. The extrapolated value for $S(0)$, including both transitions, is determined to be 0.211 ± 0.016 eV b [1]. At low temperatures, relevant to deuterium abundance sensitivity, the reaction rate for the $M1$ transition plays a significant role, contributing approximately 11

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Presenter: Do Huy Tho

P.8 – Poster, VCTP-49

Anharmonic EXAFS signals of Pb analyzed based on quantum anharmonic correlated Einstein model

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Anharmonic expanded X-ray absorption fine structure (EXAFS) signals of Lead metal (Pb) have been analyzed based on the quantum anharmonic correlated Einstein (QACE) model. This model is perfected based on the correlated Einstein model and quantum-statistical perturbation theory using an effective potential method. The effect of thermal disorders on anharmonic EXAFS signals is derived from the thermal vibrations of all atoms, with each thermal vibration quantized and treated as a phonon, and the anharmonicity is the result of phonon-phonon interactions. The obtained expressions can satisfy all their fundamental properties in the temperature dependence. The numerical results of Pb agree well with those obtained from the experimental data and other methods at various temperatures ranging from 0 K to 600 K. The obtained results show that the present QACE model can efficiently analyze anharmonic EXAFS signals of Pb from 0 K to just before the melting point.

Presenter: Tong Sy Tien

P.9 – Poster, VCTP-49

The astrophysical S-factor from proton-deuteron radiative capture within potential model

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The proton-deuteron radiative capture reaction significantly impacts primordial nucleosynthesis. The astrophysical S-factor is calculated using the phenomenological potential model for both electric dipole ($E1$) and magnetic dipole ($M1$) transitions. The results are validated against experimental data using a χ^2 test, highlighting the significance of the $M1$ transition at low energies. The obtained astrophysical S-factor [1] is in good agreement with recent results, especially the experimental data reported by Mossa et al. [2].

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Presenter: Dao Nhut Anh

P.10 – Poster, VCTP-49

Applying of complex scaling method to analyze the resonances in the weakly-bound nuclei

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Resonances are represented as the poles of the S-matrix on the complex energy plane. However, The position of the real part of the S-matrix poles does not always reflect the position of the peak of cross-sections or strength function [1,2]. The relationship between S-matrix poles and peak positions is intricate because the Jost function [3,4] is essentially a multivalued function of complex energy, so there can be energy shifts caused by the nature of the multivalued function, and if several poles exist in close proximity to each other, there is a superposition of the contributions of the individual poles. There are also background contributions arising from non-resonant continuum state contributions, because interference effects, including Fano effects, also affect the peak structure. The complex scaling method is well known as a method which can decompose the solution contribution of the S-matrix poles in the strength function and cross-sections. In this study, we apply this approach in the framework of the Jost function method. Our primary results show that by considering the asymptotic behavior of regular solutions at the poles, we can understand why the complex scaling method can distinguish and separate non-resonant continuum and resonant states.

Presenter: Trần Diệu Thùy

P.11 – Poster, VCTP-49

Study of adsorption effects of acetone and acetonitrile on defected Penta-PdSe2 nanoribbons

Nguyen Hai Dang (1,2), Pham Thi Bich Thao (1), Vo Khuong Dien (3,4), Do Minh Hoat (5,6), Nguyen Duy Khanh (7,8) and Nguyen Thanh Tien (2)

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This work employs Density Functional Theory (DFT) calculations to investigate the structural and electronic properties of ZZ7 p-PdSe2 nanoribbons (ZZ7) with various vacancy defects. Specifically, the nanoribbons exhibit excellent thermal stability, evidenced by significantly negative formation energies of around -3.9 eV. This suggests their ability to maintain stability even at high temperatures. Different vacancy defect types result in diverse geometric configurations, highlighting the structural diversity among them. Particularly, the ZZ7-V2Se structure stands out with enhanced features, especially in its strong adsorption capability for acetone and acetonitrile. Initially, ZZ7 nanoribbons exhibit nonmagnetic metallic behavior. However, the introduction of vacancy defects alters their electronic properties: ZZ7-VPd and ZZ7-VSe show ferromagnetic half-metallic band structures. ZZ7-VPd+Se and ZZ7-V2Se exhibit ferromagnetic semi-metallic band structures. The ZZ7-V2Se structure is identified as a highly effective substrate for acetone and acetonitrile adsorption, with significant adsorption energies observed -1.2 eV for acetone and -0.86 eV for acetonitrile, indicating strong adsorption capabilities. The adsorption of acetone and acetonitrile is characterized as physisorption, involving no chemical bond formation. Post-adsorption, significant changes in electronic properties are observed in ZZ7-V2Se , transitioning from ferromagnetic semi-metallic DOS to ferromagnetic half-metallic

DOS for ZZ7-V2Se-acetone-8 and ferromagnetic semiconducting DOS for ZZ7-V2Se-acetonitrile-11. These detailed findings provide a comprehensive understanding of acetone and acetonitrile adsorption on the promising ZZ7-V2Se structure, offering valuable insights for practical applications in nano-sensor technologies.

Presenter: Nguyễn Hải Đăng

P.12 – Poster, VCTP-49

Analyzing the relationship between population size and the dimension in the problem of nuclear reactor fuel reload optimization using the SHADE method

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This report explores the relationship between population size and dimension in the in-core fuel management (ICFM) problem for nuclear reactors, using the discrete Success-History based Adaptive Differential Evolution (SHADE) method. The SHADE method has been implemented for the ICFM problem of the DNRR research reactor and the VVER-1000 reactor. The ICFM problem of the DNRR comprises 100 dimensions and that of the 1/6th VVER-1000 MOX core consists of 28 dimensions. The results indicate that the optimal population size is contingent upon the problem's dimensions. For the high-dimensional DNRR reactor, a smaller population size proves beneficial, whereas the low-dimensional VVER-1000 reactor requires a larger population size. A comparison has been conducted between the objective parameters of the optimal cores obtained from the SHADE search process and those of the reference core.

Presenter: Phan Thi Thuy Giang

P.13 – Poster, VCTP-49

Classification of the Mott transitions in multicomponent fermion systems

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Metal-insulator transitions in an asymmetric three-component Falicov-Kimball model are investigated within the two-site dynamical mean field theory. The model is obtained from the symmetry breaking of the SU(3) Hubbard model by imbalanced masses and nonequal local interactions of particle components. The Mott transitions are classified by the change in the number of distinct kinds of doublons across the transition. We observe a different Mott transition between partially localized states in which the particle components (flavors), which form the doublons, are swapped with each other but the number of distinct kinds of doublons is unchanged across the transition. The swap Mott transition occurs as a result of the competition between the Brinkman-Rice and the Falicov-Kimball localizations and the mass imbalance of the mobile particles.

[Ref.: D.-A. Le, T. -M. T. Tran, M.-T. Tran, Physical Review B 109, 115105 (2024).]

Presenter: Trần Minh Tiến

P.14 – Poster, VCTP-49

The transfer of quantum entanglement in a rhombic 1/2 spins system

Vinh Le Duc

Tinh Gia 3 high school

The ability of generation and transfer of entanglement in 1/2 spins cluster opens a new direction for using spins as qubits that are the basic element of quantum computation. The generation and transfer of quantum entanglement will be investigated in a system that consists of 4 spins coupled by Ising interaction. High fidelities of quantum transfer in various directions will also be shown.

Presenter: Le Duc Vinh

P.15 – Poster, VCTP-49

Double exchange mechanism in topological insulators

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Double exchange mechanism in topological insulators is studied. The topological insulator is modeled by the Kane-Model model. A dynamical mean field theory in a rotated spin basis is constructed. It is suitable for studying different magnetization configurations, which can be non-collinear, in and out of plane. Edge states are investigated by considering a zigzag nanoribbon of the honeycomb lattice. They reveal both the edge magnetization and helicity. It is found that the in-plane antiferromagnetism is favor, but topologically trivial. The local magnetization slightly varies, but is enhanced at the edges.

Presenter: Nguyen Hong-Son

P.16 – Poster, VCTP-49

Multiphoton absorption process of an intense electromagnetic waves in monolayer graphene under the influence of both uniform electric and magnetic fields

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In this paper, we present a comprehensive theoretical study of the influence of both uniform electric and magnetic fields on multi-photon absorption of intense electromagnetic waves (IEMW) in monolayer graphene (MLG) using the quantum kinetic equation. The electron-longitudinal optical phonon scattering mechanism is considered. Analytical expressions of the multiphoton absorption coefficient in MLG indicate a nonlinear dependence on many external parameters such as temperature, electric and magnetic field magnitudes as well as the photon energy and

intensity of IEMW. We have numerically investigated the dependence of the resonance absorption spectrum as well as the Full width at half maximum (FWHM) on temperature, electric field and magnetic field. The results show that the position of resonance peaks in the absorption spectrum depends strongly on the Landau levels, electric sub-band levels, and electric field. However, temperature does not affect the position of the resonance peaks but only increases their intensity. Furthermore, the FWHM depends on the external field according to the square root law and has only a very small variation with temperature in the MLG. In particular, the external electric field increases the probability of electron-phonon scattering, causing a blue shift in the absorption spectrum and increasing FWHM. Our calculation results are in good agreement with previous theories and experiments in limited cases

Presenter: Nguyen Dinh Nam

P.17 – Poster, VCTP-49

Solubility of Carbon Dioxide in Brine: A Molecular Simulation Study

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Anthropogenic carbon dioxide (CO2) emissions, primarily from the combustion of fossil fuels, are the leading cause of global warming and climate change [1]. Therefore, reducing atmospheric CO2 emissions is critically important. Underground CO2 storage offers a promising solution, particularly in deep saline aquifers due to their vast storage capacity and widespread distribution [2]. Ensuring the long-term stability of CO2 storage in these formations requires accurately determining the solubility of CO2 in brine. Experimentally measuring CO2 solubility in brine under subsurface conditions (high pressure and high temperature) is challenging. Molecular simulation has proven to be an effective tool for addressing these challenges [3]. However, the accuracy of these simulations depends essentially on the force fields used to model the compounds. Various force fields for CO2 and brine have been independently proposed in the literature [4-6]. In this study, we have performed Monte Carlo molecular simulations to assess the capability of combining the commonly used force fields in calculating the solubility of CO2 in brine. In addition, effects on the CO2 solubility have been investigated.

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Presenter: Nguyen Tu Khai Nam

P.18 – Poster, VCTP-49

Investigation of Debye temperature and temperature-dependent EXAFS cumulants of Zn, Zr, α-Ti, Ru and Hf metals

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In this work, the anharmonic Einstein model is developed to determine the Debye temperature and investigate the temperature effects on the extended X-ray absorption fine structure (EXAFS) cumulants of hexagonal close-packed (hcp) metals. We have derived the analytical expressions of the anharmonic effective potential, the effective force constant, the Debye temperature and the first four EXAFS cumulants as a function of axial ratio $e = c/a$. Numerical calculations have been conducted for hcp Zn, Zr, α-Ti, Ru and Hf metals up to temperature 800 K. Our findings indicate that the anharmonicity of thermal lattice vibrations significantly influences the EXAFS cumulants, particularly at high temperatures. Ru atoms have the strongest coupling force causing a phenomenon that Ru lattice shows a smaller thermal disorder, and Zn has a greater thermal disorder. Additionally, we highlight the significant contributions of thermal disorder to the mean-square relative displacement at high temperatures due to thermal lattice vibrations. Moreover, our Debye temperatures derived from the developed model align reasonably well with those reported in previous studies.

Presenter: Nguyen Thi Hong

P.19 – Poster, VCTP-49

Anisotropic exciton in two-dimensional black phosphorus in a uniform magnetic field

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

Ho Chi Minh City University of Education

Exciton in monolayer semiconductor materials is of widespread interest due to their important applications in optoelectronics. An algebraic approach to this problem has been developed for excitons in monolayer transition-metal dichalcogenides with critical results. The present work further develops this algebraic approach for excitons in another conducting material, having an anisotropic structure, the monolayer black phosphorus. This problem has a more complex structure. However, we have built an algebraic representation of the Schrödinger equation through the quantum creation and annihilation operators. Then, we constructed a basis set of wave functions and obtained analytical matrix elements concerning this basis set functions. Combined with algebraic calculations, regulated perturbation theory is applied to the problem in the presence of a magnetic field, giving results consistent with other calculations. These results are essential steps, promoting the application of the algebraic method to anisotropic two-dimensional excitons at higher-approximation orders in subsequent works.

Presenter: Lê Đỗ Đăng Khoa

P.20 – Poster, VCTP-49

Missing energy method for searching heavy neutrinos via $B^- \to \ell^- N$ decays

Nguyen Hoang Duy Thanh (1), Nguyen Anh Ky (1), Dong Van Thanh (2)

(1) Institute of Physics, VAST; (2) Duy Tan University

We generate and simulate the electron - positron collisions at Upsilon(4S) resonance, the Upsilon(4S) mesons after that decay to B^+B^- pairs, the B^- mesons decay to $\ell^- N$ which is our signal and the B^+ mesons decay generically. The corresponding beam - induced background is also simulated. To minimize the sensitivity, the full event reconstruction algorithm with hadronic tag is performed to reconstruct the B^+ mesons in the interaction region. With the known information from B^+, the missing mass, which is theoretically the mass of the heavy neutrino N, can be reconstructed and utilized to search for the N. A set of selections and cuts is applied to reduce the background. The analysis and results are presented in the Poster. It shows the results of the simulation with the heavy neutrino N mass at 3 GeV after those selections and cuts, the background significantly decreases and the missing mass distribution has a peak around the value of the mass of the N, which is expected with high resolution.

Presenter: Nguyen Hoang Duy Thanh

P.21 – Poster, VCTP-49

Metal-insulator phase diagram in the ionic Hubbard model with Coulomb disorder

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(1) Institute of Physics, VAST; (2) Hanoi National University of Education

We study the metal-insulator transitions in the half-filled ionic Hubbard model with Coulomb disorder by the typical medium theory using the equation of motion method as an impurity solver. In addition to the three phases showed up in the usual ionic Hubbard model, the phase diagram of this model contains a disordered Mott insulator phase, where the geometrical averaged local density of states in the Fermi level equals zero while the arithmetical one is non-zero.

Presenter: Yen Thi Hai Nguyen

P.22 – Poster, VCTP-49

Dark charge: Probing neutrino mass and dark matter

Phung Van Dong

Phenikaa Institute for Advanced Study, Phenikaa University, Yen Nghia, Ha Dong, Hanoi, Vietnam

I show that neutrino mass and dark matter can be explained in a gauge framework for only right-handed neutrinos $\nu_{1,2,3R}$. This theory assigns $\nu_{1,2,3R}$ an abelian dark charge to be D=0, -1, and +1, respectively. It also imposes an inert Higgs doublet η and two Higgs singlets ξ, ϕ with dark charge D=+1, -1, and +2, respectively. Hence, the dark charge is broken by ϕ down to a dark parity $P_D = (-1)^D$, for which $\nu_{2,3R}$, η, and ξ are odd, whereas all other fields are even. The lightest of the odd fields is stabilized by P_D, responsible for dark matter. Neutrino masses are induced by a scotoseesaw, in which the seesaw part is mediated by ν_{1R}, while the scotogenic part is mediated by $\nu_{2,3R}$. Hence, the hierarchy of atmospheric and solar mass splittings is explained by those between the tree-level and loop-level contributions.

Presenter: Phung Van Dong

P.23 – Poster, VCTP-49

Magnetic and magneto-caloric investigation of amorphous systems in the description of disordered Ising model

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The amorphous system's magnetic properties are examined using effective field theory for the disordered Ising model with binary probabilities p for the greater ferromagnetic interaction J_1 and $(1-p)$ for the weaker ferromagnetic interaction J_2. Without an external field, we successfully produce the phase diagram which describes the critical temperature τc for ferromagnetic-paramagnetic phase transition depending on model parameters, probability p, and interacting fluctuation Δ. The linear and non-linear behavior of these $\tau_c - \Delta$ curves obtained in various experiments for amorphous ribbons are well explained in the description of our models. Besides, we analyze deeply magnetocaloric effects under the influence of external fields such as magnetic entropy change consistent with experimental observations for various amorphous systems.

Presenter: Bach Giang

P.24 – Poster, VCTP-49

A qualitative investigation of electrical conductivity in three-layer graphene structures

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We study the electrical conductivity $\sigma_1, \sigma_2, \sigma_3$ of a three-layer graphene system made of parallel-placed bilayer graphene layers. This investigation consists of three steps: The first step is calculating the effective interactions W_{11}, W_{22}, W_{33} between impurities and electrons by using the multi-component random phase approximation. The second step is defining the dependence of W_{11}, W_{22}, W_{33} on interlayer distance d, dielectric constant $\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4$, and temperature T. The third step is identifying the proportional relation between W_{11}, W_{22}, W_{33} and $\sigma_1, \sigma_2, \sigma_3$. Based on the obtained results, we deduce the rules of change of $\sigma_1, \sigma_2, \sigma_3$ when $d, \varepsilon_1, \varepsilon_2, \varepsilon_3$, and T vary.

Presenter: Le Thi Kieu Oanh

P.25 – Poster, VCTP-49

The three-level optical Stark effect of exciton in GaAs disk-shaped quantum dots

Le Thi Dieu Hien (1), Le Thi Ngoc Bao (1), Duong Dinh Phuoc (2), Dinh Nhu Thao (3)

(1) University of Sciences, Hue University; (2) Hai Ba Trung High School; (3) University of

Education, Hue University

In the framework of the effective mass approximation, the three-level optical Stark effect of exciton in the disk-shaped quantum dots is theoretically studied using the renormalized wave-function method. The characteristics of this effect are investigated through the interband optical transition rate between the two lowest levels of hole and electron in a strong pump laser field. Our numerical results and quantitative analysis not only confirm the existence of the optical Stark effect in the considered structure but also show that both the detuning, confined frequency and the geometrical parameters of the quantum dot have a strong influence on the behaviors of the exciton absorption spectrum.

Presenter: Le Thi Dieu Hien

P.26 – Poster, VCTP-49

Excitonic systems in two-layer 2D parabolic quantum dots

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In this work we consider excitonic systems such as excitons, trions and quadrons in two-layer 2D parabolic quantum dots, where electrons and holes confined in separate layers of quantum dots using an unrestricted Hartree-Fock method. The matrix elements of the Coulomb interactions between electrons and holes are derived analytically including the distance between two layers as a system parameter. The binding energies of the excitonic systems, calculated as functions of the system parameters, such as the distance between two layers, mass and confinement ratios between electrons and holes, show us the role of each kind of parameters in their overall competition picture.

Presenter: Nguyen Hong Quang

P.27 – Poster, VCTP-49

Quantum simulation of collective neutrino oscillations

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(1) Faculty of Physics, Hanoi National University of Education; (2) Faculty of Computer Science and Phenikaa Institute for Advanced Study, Phenikaa University

It is well known that in extreme astrophysical environments, the neutrino flavor changes due to three factors: vacuum oscillations, interactions with surrounding matter, and collective oscillations resulting from interactions between different neutrinos. In this work, we present the quantum simulation of a small system of interacting neutrinos using a quantum computer.

Presenter: Vũ Văn Hướng

P.28 – Poster, VCTP-49

Hydrodynamic simulation of the air flow and dust particle motion in a multi-stage impactor

Pham Tuan Kiet (1), Dinh Van Trung (1,2)

Institute of physics, VAST

Multi-stage impactors have been widely used to collect atmospheric aerosols and separate them into size bins. In this contribution, we study the working of a real multi-stage impactor using publicly available hydrodynamic simulation code OpenFoam. We determine the steady state air flow inside the multi-stage impactor and then calculate the trajectories of the aerosol particles with different sizes within the Lagrangian framework. Using the simulation results, we estimate the collection efficiency of each impactor stage. We also compare the simulation results with the size distribution of the aerosols collected using our multi-stage impactor.

Presenter: Pham Tuan Kiet

P.29 – Poster, VCTP-49

Thermal-Magnetic Effect on the Excited-State Energy Levels of a Plasma-Embedded Hydrogen Atom in a homogeneous Magnetic Field

Gia-Phu Huynh (1), Huong-Giang T. Nguyen (1), Thanh-Truc H. Nguyen (2) and Duy-Nhat Ly (1)

(1) Ho Chi Minh City University of Education, Vietnam; (2) Marie Curie High School, Ho Chi Minh City, Vietnam.

Energy spectra of a plasma-embedded hydrogen atom in a homogeneous magnetic field is a topic of great interest in plasma physics [1–7]. In this paper, we investigate the simultaneous influence of thermal motion of the center of mass and the magnetic field on the energy spectra, referred to as the thermal-magnetic effect. Currently, it is possible in the laboratory to create a stable magnetic field with an intensity of about 100 Tesla for a long enough time for investigation [6] and to create plasma with a temperature of several MeV [7]. Therefore, in addition to studying the influence of the magnetic field on the energy spectra of hydrogen atoms in plasma, it is necessary to investigate the thermal motion of the electron-nucleus center of mass in the magnetic field. This influence is taken into account because the term $-\frac{e}{M}(\mathbf{B}\times\mathbf{K})\cdot\mathbf{r}$ appears in the Hamiltonian, which is accurately separated from the center of mass [1,2]. Here, $\mathbf{K}$ is the pseudo-momentum vector of the center of mass related to the temperature according to the Maxwell–Boltzmann distribution $\overline{K^2} = 3Mk_BT$. We use perturbation theory to study this effect of simultaneous temperature and magnetic field influences on the spectra and wavefunction. For the first excited state, the energy shift is 0.2.

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Presenter: Ly Duy-Nhat

P.30 – Poster, VCTP-49

Low Energy Levels of Excitons in Monolayer TMDs in a Homogeneous Magnetic Field Using the FK Operator Method

Vinh-Phat Tran (1), Huu-Duc Le (1), Thu-Ha N. Luong (1) and Duy-Nhat Ly (1)

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The energy spectra emitted from Monolayer Transition Metal Dichalcogenides (TMDs) in a homogeneous magnetic field have been studied extensively through both theory and experiment [1–4]. By comparing theoretical and experimental energy spectra, structural information about TMDs, such as reduced exciton mass, polarizability, and the dielectric constant of the surrounding medium, can be retrieved [1,4]. This information is crucial for understanding the properties of TMDs. In this paper, the Keldysh interaction potential is written in the standard form of the creation operator and annihilation operator through Fourier transformation. From there, the exact matrix element expression is found using the Feranchuk–Komarov (FK) operator method [5]. Analytical energy levels of 1s, 2s and 3s states, depending on the magnetic field, are compared with experimental values [4]. The results show that in the ground state and low excited states in the low magnetic field region, the error is below In the magnetic field region higher than 40 Tesla, the 3s level has error of less than Although the theoretically calculated energies are currently limited to zero-order perturbation, the results demonstrate the effectiveness of applying the FK operator method with the Fourier transformation. This result will be developed further at higher perturbation orders to achieve analytical solutions that are in closer agreement with experimental data.

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Presenter: Le Huu Duc

P.31 – Poster, VCTP-49

Thermoelectric and magnetic properties of bismuth telluride with a Gd point defect

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Rare earth-doped Bi2Te3 reveals many exotic magnetic properties promising for functional-material applications such as thermoelectricity and spintronics. In this work, we carried out first-principles electronic structure calculation within the density functional theory to examine the magnetic and thermoelectric properties of the bismuth telluride with a Gd point defect. The newly formed compound Gd1/3Bi5/3Te3, composed of a Te-Gd-Te-Bi-Te layer sandwiched between two quintuple layers, is ferromagnetic with a magnetic moment of 7.0 μB. This value originates from the f-states of Gd inside the layer. The Te-Gd-Te-Bi-Te layer leads to the semimetallic behavior of the compound. The feature enhances the bipolar conduction effect, reducing the power factor. Optimizing the carrier concentration and keeping temperatures low are methods to improve the thermoelectric performance of Gd1/3Bi5/3Te3

Presenter: Tran Van Quang

P.32 – Poster, VCTP-49

Investigating the damping states of drift velocity of electrons in GaAs semiconductor under the influence of external electric field

Nguyen Phuoc The (1,2), Le Thi Thu Thuy (2)

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This article presents the results of investigating the damping states of drift velocities of electrons in GaAs semiconductor with p-i-n structure using the Ensemble Monte Carlo (EMC) method under the influence of an external electric field. The selected device model has a pure semiconductor layer (i) in the middle with a size of several hundred nanometers, two semiconductor layers p and n on both sides with the same size chosen to be 20 nm, the photocarrier which was created by Ultra-fast laser pulses in the direction from p to i and then n layer with a concentration of about $10^18cm - 3$ Simulation results show that, when there is no external electric field, under the influence of the internal electric field due to the uneven distribution of carriers in the device, the velocity of electrons in the device is gradually damped, as observed in previous studies. With a specified size of the pure semiconductor layer, we used the external electric field as a control parameter. Gradually increasing the electric field every intervals of 20kV/cm resulted in a transition in the velocity state from under the damping to the crictical damping limit and then over the damping. Investigations with different sizes enabled us draw a phase diagram in the phase space between the critical electric field (EC) and the size (S) of the pure semiconductor layer. In addition, the research results also show that this critical electric field depends heavily on the concentration of the exciting carrier. The higher the temperature, the lower the critical electric field, while the higher the carrier concentration, the higher the critical electric field value.

Keywords: Damped oscillation, EMC simulations, p-i-n structure, GaAs semiconductor

Presenter: Thùy Thị Thu Lê

P.33 – Poster, VCTP-49

Questions of flavor physics and neutrino mass from a flipped hypercharge

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The flavor structure of quarks and leptons is not yet fully understood, but it hints a more fundamental theory of non-universal generations. We therefore propose a simple extension of the Standard Model by flipping (i.e., enlarging) the hypercharge $U(1)_Y$ to $U(1)_X \otimes U(1)_N$ for which both X and N depend on generations of both quark and lepton. By anomaly cancellation, this extension not only explains the existence of just three fermion generations as observed but also requires the presence of a right-handed neutrino per generation, which motivates seesaw neutrino mass generation. Furthermore, in its minimal version with a scalar doublet and two scalar singlets, the model naturally generates the measured fermion-mixing matrices while it successfully accommodates several flavor anomalies observed in the neutral meson mixings, B-meson decays, lepton-flavor-violating decays of charged leptons, as well as satisfying constraints

from particle colliders.

Presenter: N. T. Duy

P.34 – Poster, VCTP-49

Negative Poisson's ratio and anisotropic carrier mobility in ternary Janus Si_2XY (X/Y = S, Se, Te): First-principles prediction

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In this report [1], the structural, mechanical, electronic, and transport properties of two-dimensional (2D) ternary Janus Si_2XY (X/Y = S, Se, Te) monolayers are studied based on the calculations using first-principles density functional theory. All three structures are found as direct semiconductors with moderated bandgap energies and good stabilities for experimental synthesis. The transport properties are also examined by calculating the carrier mobilities. We find that the carrier mobilities of all three monolayers are anisotropic not only between the electrons and holes but also between the two transport directions. The $Si_2$2SSe monolayer exhibited the highest electron mobility of 897.66 cm^2/Vs in the x axis. Amazingly, our calculations reveal that the Si2XY monolayers are auxetic materials with negative Poisson's ratio along both x and y axes. Particularly, the $Si_2$2SSe has the largest negative Poisson's ratio value of -0.131 in the x direction. These obtained results open more prospects for advanced applications of these materials in electronics, optoelectronics, and nanomechanics.

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Presenter: Hieu Ngoc Nguyen

P.35 – Poster, VCTP-49

Distribution of the electric field inside an optical microcavity for different input angles

Le Tri Dat (1,2), Vinh N.T. Pham (3), and Nguyen Duy Vy (4,5)

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Calculating the electric fields is crucial for determining several important physical parameters in many optical devices. Our recent work examined the optical absorption of a graphene film inside an optical microcavity by analyzing the electric field distribution through various dielectric environments, with the input laser source aligned perpendicular to the propagation direction. Practically, many studies have focused on investigating the optical absorption of absorber materials at different incident angles. These open up numerous questions related to controlling light-nanoobject interactions in optical systems, particularly within an optical microcavity. In this study, we focus on computing the electric field distribution in the resonant cavity under different incident angles. This approach provides a clearer understanding of the field distribu-

tion within the optical cavity and facilitates further calculations on the optical absorption of graphene sheets.

Acknowledgement: This work is supported by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under the grant number 103.01-2023.36.

Presenter: Le Tri Dat

P.36 – Poster, VCTP-49

Systematic investigation on pairing phase transition in excited nuclei

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The pairing phase transition in excited nuclei is systematically investigated by using the experimental nuclear level densities (NLDs) which have been compared with those obtained within the phenomenological back-shifted Fermi-gas (BSFG) model. The heat capacity is carried out by taking into account the experimental nuclear level density (NLD) data measured using the Oslo method for the low-excitation region below the neutron binding energy B_n combining with the BSFG NLD model for the excitation energy from B_n to about 120 MeV. The S-shape observed in the heat capacity of both even-even and even-odd isotopes gives a precise description of the pairing phase transition in nuclei. However, the S-shape exhibited is different not only between even-even and even-odd isotopes but also depends on the neutron number.

Presenter: Le Thi Quynh Huong

P.37 – Poster, VCTP-49

Nonlinear oscillator model of experience-based decisions and application of normal distribution on Hanoi high school entrance exam grading

Chu Thuy Anh

Institute of Physics, Vietnam Academy of Science and Technology

Experience-based decision making might affect final results on several topics. Previous experiences/ results contribute as one of the main parameters in decision making, leads to oscillation of the final results between several scenarios. In this work, a nonlinear oscillator model is proposed to describe the affects of experience-based decision as external forces, probably leads to the chaotic behavior of final results. An investigation on Hanoi high school entrance exam marks is used an an illustration, accomplish with normal distribution to examine the accuracy of the exam along the time.

Presenter: Chu Thuy Anh

P.38 – Poster, VCTP-49

Dynamical properties of photon-added squeezing-enhanced coherent state in the Jaynes-Cummings model

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In this paper, we study the dynamical properties of a recently introduced state called photon-added squeezing-enhanced coherent state (PASECS). We investigate the time evolution of the probabilities and the second-order correlation functions of this state. Our findings indicate that the dynamical behaviors of the field in the PASECS differ significantly from those of the field in the original coherent state. The results reveal that the dynamical properties are affected by variations in the photon addition and the squeezing-enhanced parameters.

Presenter: Le Thi Hong Thanh

P.39 – Poster, VCTP-49

Efficient qutrit gates in superconducting circuits using quantum optimal control

Tuan-Kha Tran (1), Van-Duy Nguyen (2)

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The implementation of qutrit gates in superconducting circuits presents a promising avenue for enhancing the computational power of quantum processors. This study explores the development and optimization of efficient qutrit gates using quantum optimal control techniques. By leveraging the additional state offered by qutrits, we aim to increase the computational density and reduce error rates in quantum computations. We employ state-of-the-art quantum optimal control methods to design pulse sequences that achieve high-fidelity qutrit gate operations in superconducting circuits. Our approach demonstrates significant improvements in gate performance, robustness against decoherence, and scalability. The results offer a pathway towards more powerful and error-resilient quantum computing architectures, paving the way for advanced quantum algorithms and applications.

Presenter: Tran Tuan Kha

P.40 – Poster, VCTP-49

A very low bandgap line-tunnel field effect transistor with channel-buried oxide and laterally doped pocket

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Low bandgap and line tunneling techniques have demonstrated the most effectiveness in enhancing the on-current of tunnel field-effect transistors (TFETs). This study examines the mechanisms and designs of channel-buried oxide and laterally doped pocket for a very low bandgap line-TFET. Numerical TCAD simulations show that the channel-buried oxide is needed to prevent the off-state lateral tunneling while still maintaining the on-state vertical tunneling. The buried oxide pillar should be high so that the channel is thin about 10 nm thickness to completely suppress the tunneling leakage. The dopant pocket is required to trigger the line tunneling earlier than the point tunneling to improve the subthreshold swing and on-current. Increasing the pocket concentration or decreasing the pocket thickness both cause an increase not only in the vertical band bending but also in the effective gate-insulator thickness. Because of the trade-off between these two operation parameters, for a given thickness/concentration, there exists an

optimal concentration/thickness of the pocket to maximize the on-current. The on-current is optimized using a heavy and thin pocket for which the band bending is maximized and the effective gate-insulator thickness is minimized. For the fabrication feasibility using existing doping techniques, the pocket concentration and thickness should be respectively 10^{19} cm^{-3} and 4 nm to maximize the on-current of the InAs line-TFET.

Presenter: Nguyễn Đăng Chiến

P.41 – Poster, VCTP-49

Nonlinear multi-photon Absorption of a Strong Electromagnetic Wave with electron-acoustic phonon scattering in infinite semi-parabolic Plus semi-inverse Squared Quantum Wells .

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Theoretical study of the nonlinear multi-photon absorption of a strong electromagnetic wave in infinite semi-parabolic plus semi-inverse Squared Quantum Wells (ISPPSISQW) by using quantum kinetic equations for the case of electron-acoustic phonon scattering. Analytical expressions for the nonlinear multi-photon absorption coefficient in the ISPPSISQW are obtained for a specific GaAs/GaAsAl in the case of the absence and the case of the presence of an external magnetic field B. A second-order multi-photon process is included in the result. The dependence of the nonlinear multi-photon absorption coefficient on the intensity E_0 and the frequency Ω of a strong electromagnetic wave, confinement frequency of ISPPSISQW ω_z and the temperature T is investigated. The numerical computations for a specific ISPPSISQW GaAs/GaAsAl show that the nonlinear multi-photon absorption coefficient decreases rapidly with increasing ω_z or Ω and the nonlinear multi-photon absorption coefficient increases rapidly with E_0 or T. In the case of the presence of an external magnetic field B, the Shbnikov- de Hass (SdH) oscillations have appeared in the dependence of the nonlinear multi-photon absorption coefficient on the magnetic field B. The amplitude of the SdH oscillations in the absorption coefficient decreases as the system's temperature T increases, and the amplitude of the SdH oscillations in the absorption coefficient will increase as the frequency Ω increases.

Presenter: Dung Thi Bui

P.42 – Poster, VCTP-49

Quantum Computing with Cat qubits

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Cat qubits leverage a continuous-variable quantum error correction code. The phase of the coherent states can be corrected using an appropriate feedback mechanism, and any bit-flip errors that do occur can be detected and corrected with high probability. In this work, we investigated the dynamics of the cat qubit driven by a microwave pulse.

Presenter: Tran Thi Thanh Huyen

P.43 – Poster, VCTP-49

Mass imbalance effects on microcavity exciton-polariton condensates

Thi-Hau Nguyen(1,2), Thi-Hong-Hai Do(2) and Van-Nham Phan(3)

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The interplay of the excitonic, polaritonic and photonic condensation states due to the mass difference of electrons and holes in a microcavity is examined. In the framework of the unrestricted Hartree-Fock approximation adapting to the two electronic bands with the electron-hole Coulomb attraction and light-matter coupling, we find a set of self-consistent equations evaluating the order parameters of the condensation states. The excitonic and the photonic susceptibility functions are also specified in the random phase approximation. Our numerical results release the polaritonic condensate dominance at low excitation densities once enlarging the mass imbalance. The excitonic, polaritonic and photonic condensate competition in the influence of the Coulomb interaction and mass imbalance is also discussed

Presenter: Nguyen Thi Hau

P.44 – Poster, VCTP-49

Thermodynamic properties of monolayer honeycomb spin lattice

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The transverse Ising model is used in the thermodynamic theory of ferroic materials [1]. The Ising model in longitudinal field is used to investigate the first order magnetization process in bilayer honeycomb spin films [2]. In this research, spin systems with arbitrary spin value S in a single-layer honeycomb spin lattice have been investigated using the functional integral method and the Ising model in longitudinal and transverse fields. An expression for the free energy in the Gaussian approximation consisting of two terms has been obtained: the mean field term and the spin fluctuation term. From this, expressions for the general spin wave spectrum for different magnetic structures (ferromagnetic, antiferromagnetic, and ferrimagnetic) have been obtained. The influence of spin fluctuations on the magnetization process in an external field for a ferromagnetic structure has been examined.

References:

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Presenter: Nguyen Tu Niem

P.45 – Poster, VCTP-49

W Mass Anomaly and Physics Beyond the Standard Model

Dao Thi Nhung

Phenikaa University

In this talk I will present the 7 standard deviation discrepancy between the W mass measured by the CDF collaboration in 2022 and the Standard Model prediction. This anomaly can be explained in models beyond the Standard Model and I will discuss an example of such models.

Presenter: Đào Thị Nhung

P.46 – Poster, VCTP-49

Influence of cut-off frequency effect on resonance energy transfer and Casimir-Polder interaction

Nguyen Dung Chinh (1,2), Vinh Nguyen Thanh Pham (3,4), and Nguyen Duy Vy (5,6)

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Using the Green's function approach, we study the resonance energy transfer (RET) rate between two parallel identical two-level atoms in the presence of three types of cylindrical system: a distributed Bragg reflector (DBR), a perfectly reflecting wall (PRW), and a two-layer silicon fiber. Upon applying the cut-off frequency condition, our analysis reveals a profound suppression in the RET rate for atoms positioned along the axis of the cylinder with the PRW. Conversely, for atoms situated within the DBR, the results demonstrate enhancement in the far zone. Furthermore, it is shown that when two atoms oriented radially are placed inside and near the surface of the silicon fiber, the RET rate is completely inhibited. We also investigate the Casimir-Polder (CP) interaction between a cut-off-frequency DBR and an excited atom. A fully attractive potential towards the surface of the DBR is found for the atom inside the waveguide.

Presenter: Nguyen Dung Chinh

P.47 – Poster, VCTP-49

Magneto-optical absorption properties of monolayer transition metal dichalcogenides including electron-phonon interaction

Tran N. Bich (1,2), Le T. Hoa (3), Le Dinh (3), and Huynh V. Phuc (1)

(1) Dong Thap University; (2) Quang Binh University; (3) University of Education, Hue University

We study how the electron-phonon interaction (EPI) affects the reliance of the linear and nonlinear magneto-optical absorption coefficients (MOACs) and refractive index changes (RICs) on the external electromagnetic field and electron spin orientation in monolayer MX_2 (M=Mo/W, X=S/Se) semiconductors. This work relies heavily on the density matrix method as its main

research tool. The results show that the EPI effect reverses the variation of MOACs absorption peak intensity according to changes in the external fields and spin state of electron. This effect enhances the influence of the external field on RICs absorption peak intensity. We observe that control over the optical properties of MX_2 monolayers is achievable through adjustments in the external field value. This versatility is highly desirable for advanced materials.

Presenter: Trần Ngọc Bích

P.48 – Poster, VCTP-49

First-principles prediction of the Ohmic contact and ultralow Schottky contacts in two-dimensional metal-semiconductor van der Waals heterostructures

Chuong V. Nguyen (1), Cuong Q. Nguyen (2), Nguyen N. Hieu (2), Nguyen V. Hieu (3)

(1) Le Quy Don Technical University; (2) Duy Tan University; (3) Danang University of Education.

Electrical metal-semiconductor (M-S) contacts between metals and semiconductors are widely used in modern electronic devices. These contacts form the basis of many device architectures and are crucial for the operation of many electronic devices. At the interface of the M-S contact, an interfacial potential barrier, referred to as the Schottky barrier (SB), is typically formed. In electronic devices, a significant Schottky barrier height (SBH) can significantly hinder the charge injection efficiency. Since the SBH is closely associated with the contact resistance at the M-S contact, reducing the SBH at the M-S contact has become a significant challenge in achieving next-generation electronics technology. Therefore, it is crucial to develop effective contact engineering approaches to form either Ohmic contacts or ultralow Schottky contacts, which are highly preferred for approaching the intrinsic characteristics of 2D devices. In this work, by performing first-principles calculations we designed several M-S heterostructures between 2D metals (MoSH, Graphene) and 2D semiconductors (MoSi2N4, BSe) [1, 2]. Our findings could provide a new pathway for the design of high-performance electronic devices based on these 2D M-S heterostructures.

References:

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[2] Langmuir 39 (2023) 6637–6645

Presenter: Nguyễn Văn Chương

P.49 – Poster, VCTP-49

Investigation of C and Si-doped 2D germanene quantum dots for potential nanotechnology applications

Hoang Van Ngoc

Thu Dau Mot University

Research on nanostructured materials underpins the development of contemporary smart devices. This study focuses on pristine 2D germanene quantum dots and their carbon (C) and silicon (Si) doped counterparts. The investigated structures are monolayers, each comprising 37 germanium (Ge) atoms with hydrogen-passivated edges. Density functional theory (DFT), coupled with the Vienna Ab initio Simulation Package (VASP), was employed for the analysis. The findings reveal that all three structures are stable and exhibit non-magnetic metallic properties. Notably, C-doping significantly reduces the buckling height of the system. Systematic exami-

nation of the partial densities of states indicates complex multi-orbital hybridizations. Charge density difference analysis demonstrates a decrease in charge around C atoms and an increase around Si atoms. This research enhances the understanding of germanene materials and lays the groundwork for their potential applications in nanotechnology.

Presenter: Hoang Van Ngoc

P.50 – Poster, VCTP-49

Isospin mixing in the nuclear low-lying resonances

Le Tan Phuc

Institute of Fundamental and Applied Sciences, Duy Tan University

Since its introduction by Heisenberg in 1932 [1], the Isospin concept has proven highly effective in describing nuclear systems. From this concept emerged a new symmetry known as isospin symmetry. However, the influence of the Coulomb field breaks this symmetry, resulting in the mixing of states with different Isospins and thus isospin is no longer a good quantum number. Notably, in the low-lying tail of nuclear giant dipole resonances (GDR), isospin mixing is observed, particularly in the Pygmy dipole resonances (PDR) region. This report examines the variation of PDR concerning temperature and isospin mixing that occurs in this region.

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Presenter: Le Tan Phuc

P.51 – Poster, VCTP-49

Quantum Circuit Ansatz Structures for Ising Model & A Comparative Analysis of Classical and Quantum Optimization Methods

Lê Dức Truyền (1,2), Nguyễn Vũ Linh (3), Nguyễn Văn Duy (2), Nguyễn Quốc Hưng (4), Nguyễn Công Hà (5), Hà Triết (6)

(1) National Tsing Hua University; (2) Phenikaa University; (3) The Ho Chi Minh City University of Science; (4) Nano and Energy Center, VNU University of Science; (5) École normale supérieure - PSL; (6) Rhodes College

In this study, we conducted a detailed study of several different kinds of quantum circuit ansatz structures in order to find the one that would work best with the Ising model and Noisy Intermediate Scale Quantum Computing (NISQ), which we utilized the symmetry of the investigated model. Additionally, we also delved into several optimization methods, both classical and quantum, and analyzed the quantum advantage that each of these methods offered, and then we proposed a new combinatorial optimization scheme, deemed as QNSPSA-PSR which combines calculating approximately Fubini-study metric (QNSPSA) and the exact evaluation of gradient by Parameter-Shift Rule (PSR). The QNSPSA-PSR method integrates the QNSPSA computational efficiency with the precise gradient computation of the PSR, improving both stability and convergence speed. Our results provide a new potential quantum supremacy in the VQE's optimization subroutine and enhance viable paths toward efficient quantum simulations on NISQ devices.

Presenter: Le Duc Truyen

P.52 – Poster, VCTP-49

Study of nonlinear phenomena in advanced materials and devices: insights from distinct approaches

(1) Tran Ky Vi , (2) Nguyen Viet Hung, (3) Nguyen Quang Hoc, (3) Bui Duc Tinh, (4) Nguyen Dang Quang Huy, (5) Tran Chi Quy

(1) Physics and Young Magazine, Vietnam Physics Society; Hanoi University of Science and Technology; (3) Hanoi National University of Education; (4) VNU Vietnam Japan University; (5) Hanoi-VNU University of Science

This research explores three branches of nonlinear phenomena using distinct approaches. The first branch employs the statistical momentum method for nonlinear mechanics, calculating elastic deformation properties of Fe and its alloys (FeSi, FeC, FeH), highlighting temperature and pressure dependencies. The second branch investigates nonlinear photonics through a hybrid variational method applied to the nonlinear Schrödinger equation, analyzing beam propagation and soliton interactions in graded-index optical waveguides, and validating these findings with simulations. The third branch studies superconducting materials using the time-dependent Ginzburg-Landau equation with thermal noise, modeling transport properties near the critical temperature, and demonstrating that high electric fields suppress fluctuations and maintain residual superconductivity above Tc, consistent with Sn nanowire experiments.

Presenter: Tran Ky Vi

P.53 – Poster, VCTP-49

Stability, electronic and mechanical properties of ZnO graphenylene-like nanosheet single and double layer: A first-principles study

Nguyen Thi Thao (1), Vu Ngoc Tuoc (2)

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The quest for sustainable semiconductor devices that can be utilized across diverse applications necessitates the creation of groundbreaking materials with multifunctional properties. Recently, two-dimensional (2D) nanoporous materials have garnered attention as potential functional materials due to their promising applications in areas such as energy storage, sensing, and catalysis, particularly material structures with semiconductor properties. This study presents a new family of inorganic structures based on the biphenylene network in monolayer and bilayer forms derived from zinc oxide (ZnO), which could significantly expand the repertoire of thin-layer porous materials, analogous to graphene-like nanoporous materials [1-5]. Using first-principles calculations based on density functional theory (DFT) and density functional tight-binding theory (DFTB), this research examines the energetic and mechanical stability as well as the electronic and mechanical properties of these 2D porous structures. The calculated stiffness constants and phonon spectra indicate that these structures are thermodynamically stable. Simulated ab-initio molecular dynamics (AIMD) at 300 and 400 K confirm their stability under ambient conditions. Both studied structures are wide-bandgap semiconductors with bandgap energies ranging from 4.0 to 5.3 eV. Due to their favorable electronic and mechanical properties, these nanosheets are well-suited for applications in nanomechanics and nano-optoelectronics, making them promising candidates for future technological advancements in these fields. Keywords: Nanosheet, DFT, DFTB, Graphenylen, Nanoporous sheet, Sructure design.

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Presenter: Nguyễn Thị Thảo

P.54 – Poster, VCTP-49

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 for kagome magnetic materials. In previous studies, we constructed a minimal model for kagome magnetic materials consisting of two terms. The first term describes the Heisenberg spin exchange of electrons. We consider the case where the spin exchange is isotropic in-plane but anisotropic out-of-plane. The second term is the Dzyaloshinskii-Moriya interaction. We consider the Dzyaloshinskii-Moriya interaction to be parallel to the z-axis only due to the symmetry of the kagome lattice. In this study, we will extend the above model to investigate the proposed magnetic competition in kagome magnetic materials. This model can describe the electronic dynamics in kagome magnetic materials. The model is based on the tight-binding model of itinerant electrons and the double exchange model. Using the Bogoliubov variational principle we find the ground state at zero temperature.

Presenter: Tran Thi Thanh Mai

P.55 – Poster, VCTP-49

Phenomenological Analogy between Gross-Pitaevskii Theory for Bose-Einstein Condensate mixtures in infinite space and Classical Mechanics

Pham Duy Thanh and Nguyen Van Thu

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In this work, we find an intriguing analogy between the Gross-Pitaevskii equations for binary mixtures of Bose-Einstein condensates at zero temperature and Newton's equations of motion for a particle in a conservation field within the framework of classical physics. Although this analogy is pure phenomenological, it provides us with a new perspective on physics in condensed matter physics, especially quantum matter.

Presenter: Pham Duy Thanh

P.56 – Poster, VCTP-49

AI-Powered Mie Theory for Predicting Optical and Photothermal Heating of Nanoparticles

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We introduce a novel approach combining artificial intelligence (AI) and Mie theory to investigate the optical and photothermal properties of nanoparticles. Utilizing computer vision algorithms, we analyze transmission electron microscopy (TEM) images to extract nanoparticle size, shape, and distribution data. This structural information is then integrated into Mie theory calculations to predict absorption, scattering, and extinction spectra. Furthermore, we model the photothermal heating of nanoparticles dispersed in water or polymer matrices under laser irradiation, predicting the time-dependent temperature rise based on nanoparticle concentration and illumination duration. A user-friendly web application built on Streamlit enables researchers to easily utilize our approach for custom calculations.

Presenter: Ngô Thị Quế

P.57 – Poster, VCTP-49

Machine Learning-Accelerated Design of Titanium Nitride Nanoring Metamaterial Absorbers for Broadband Solar Energy Harvesting

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Metamaterial absorbers offer immense potential for applications in solar energy harvesting, radar systems, and emerging technologies. This study presents a novel two-layer metamaterial absorber design consisting of periodic titanium nitride (TiN) nanoring arrays on a TiN substrate, achieving an average absorption of 93% across the 200-3000 nm wavelength range, with a peak absorption of 99% and a total solar absorption efficiency of 95.5% under AM1.5 illumination. Recognizing the computational challenges in optimizing such nanostructured designs, we introduce a machine learning (ML)-driven approach to accelerate the design process. Three Python-based regression models (K-Nearest Neighbors, Random Forest, and Decision Tree) are trained on simulated absorption spectra and their corresponding structural parameters. Among these, the Decision Tree model demonstrates the highest accuracy with an R2 score of 0.99, enabling rapid prediction of absorption spectra from geometric parameters. This ML-accelerated approach holds promise for significantly streamlining the design and optimization of metamaterial absorbers for a wide range of applications.

Presenter: Đặng Bùi Nhật Lê

P.58 – Poster, VCTP-49

Investigating the conditions for CO2 sensing in the p-SiC2-SS nanoribbon model using DFT simulation method

Tran Yen Mi, Huynh Anh Huy, Huynh My Linh

Can Tho University

Our previous research has shown that the p-SiC2-SS model possesses special electronic properties making it a potential a gas sensor. Using DFT simulation, we initially determined the conditions for p-SiC2-SS to capture CO2 molecules, a task that is challenging for other nanoribbon models. This preliminary result will be the premise for our further studies on the CO2 sensing capability of p-SiC2-SS.

Presenter: Tran Yen Mi

P.59 – Poster, VCTP-49

Exploring Empirical Thermodynamic Quantities of Excited Nuclei Through Canonical Ensemble

Nguyen Ngoc Anh (1,2), Tran Vu Dong (3,4), Phan Nhat Huan (3,4), Nguyen Quang Hung (3,4), Nguyen Xuan Hai (5), Le Thi Quynh Huong (6)

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Thermodynamic quantities (TQs), including the free energy, entropy, total energy, and heat capacity of excited nuclei, play important roles, as they not only contribute to clarifying the structure and properties of atomic nuclei but also serve as a connection between the microscopic realm and macroscopic domains, e.g., from the tiny world of nucleons to infinite nuclear matters. From the experimental nuclear level density (NLD) data at the excitation energy below the neutron binding energy and the back-shifted Fermi gas NLD model, we have derived semi-empirical TQs of 78 nuclei, whose mass number ranges from 43 to 243, using the canonical ensemble. The obtained results reveal four systematic conclusions, as follows: (1) The free energy of even-even nuclei exhibits distinct behavior as compared to that of odd-A ones; (2) The variation of total energy with respect to nuclear temperature demonstrates the constant temperature characteristic of nuclei at low-excitation energies; (3) The entropy undergoes sudden changes at critical temperatures of approximately 0.3 and 0.55 MeV for medium- and heavy-mass nuclei, respectively. These changes are interpreted as the break of the first Cooper pair; (4) Pronounced S-shapes are seen in the heat capacities of nuclei of rare-earth elements. In addition, the temperatures defined at the center of these S-shapes are pretty close to theoretical predictions for the critical temperature of pairing phase transition. These results have been published in [J. Phys. G: Nucl. Part. Phys. 51 (2024) 065105].

Presenter: Nguyen Ngoc Anh

P.60 – Poster, VCTP-49

Evaluation of Pafnucy deep neural network model for ligand based drug virtual screening

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Pafnucy is a 3D convolutional neural network that predicts binding affinity for protein-ligand complexes developed by Marta et. al. The original version was trained on the PDBbind database in 2016 and tested on the CASF "scoring power" benchmark. In this study, we retrain the Pafnucy model with more updated data. The Pafnucy models were then used to predict protein-ligand affinity on SARS-COV-2 and mu-opioid receptors. The calculated results show that Pafnucy models can predict the protein-ligand binding affinity very fast with a good accuracy. Our retrained Pafnucy model gives results with higher accuracy than the original version. Pafnucy has great potential when combined with traditional computational tools such as molecular dynamics and docking to speed up the virtual drug screening process.

Presenter: Nguyen Tien Cuong

P.61 – Poster, VCTP-49

Investigating the site-dependent thermal stability of G6PD by coarse-grained and all-atom simulations

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The enzyme glucose-6-phosphate dehydrogenase (G6PD) plays an important role in protecting red blood cells against oxidative damage through the production of reductive NADPH. A reduced activity of G6PD can lead to red blood cell breakdown causing hemolytic anemia. G6PD deficiency, being the most commonly known enzymopathy, is genetically inherited affecting 5% of the world population. The catalytic activity of G6PD has been shown experimentally to correlate with its thermal stability. By using molecular dynamics simulations with a coarse-grained structure-based model we have shown that residue positions (or sites) in the protein sequence that have the largest contributions to the protein's specific heat are statistically linked to point mutations associated with G6PD deficiency. Here, we dwell further into this issue by doing all-atom simulations of the monomeric G6PD in water solution. We show that the site-dependent thermal stability in the coarse-grained model to a significant degree correlates with that in all-atom simulations.

Presenter: Nguyen Thi Thuy Nhung

P.62 – Poster, VCTP-49

Vacuum stability using Vector like Quarks (VLQ)

Aman Verma, Dinesh Kumar

Department of Physics University of Rajasthan, Jaipur

We consider the Standard model extenstion by vector-like quarks and investigate the Higgs potential's vacuum stability in the presence of several vector-like quarks. Since their masses are not produced by the Higgs mechanism, vector-like quarks can have any mass in the Lagrangian and have the same coupling for both left and right handed components. We have selected seven vector-like quark representations and analyzed the contribution to renormalized group equations to gauge, yukawa and Higgs quartic coupling. Since the introduction of new vector-like quarks will alter the direction of the Higgs quartic coupling, we have examined the impact of RGE running on the vacuum stability of Higgs. We also verify the number of vector-like quark copies needed in each scenario to attain the vacuum stability of the Higgs potential.

Presenter: Aman Verma

P.63 – Poster, VCTP-49

Investigation of phase transitions of the frustrated $J_1 - J_2$ Ising model on a square lattice in magnetic fields

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The $J_1 - J_2$ frustrated Ising model on a square lattice is investigated using the functional integral method with competing interactions J_1 (nearest neighbor, antiferromagnetic) and J_2 (next nearest neighbor, antiferromagnetic). We determine the ground state of the model including Néel antiferromagnetic and stripe antiferromagnetic phases, which depend on the value of the frustrated parameter $\alpha = J_2/J_1$. For $\alpha = 0.5$, the model becomes frustrated because the ground states are infinitely degenerate and there is a discontinuous transition from the Néel antiferromagnetic phase to the stripe antiferromagnetic phase at $\alpha = 0.5$. Besides, we also discuss on the effect of spin fluctuations and of longitudinal and transverse fields on order parameters for two cases, $\alpha > 0.5$ and $\alpha < 0.5$.

Presenter: Pham Huong Thao

P.64 – Poster, VCTP-49

Neuropilin-1 protein may serve as a receptor for SARS-CoV-2 infection: Evidence from molecular dynamics simulations

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Human cell angiotensin converting enzyme 2 (ACE2) is the most popular receptor for severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), but other receptors have been observed in experiments. Neuropilin-1 protein (NRP1) is one of them, but the mechanism of its binding to the wild type (WT) and different variants of the virus remains unclear at the atomic level. In this work, all-atom umbrella sampling simulations were performed to clarify the binding mechanism of NRP1 to the spike protein fragment 679–685 of the WT, Delta, and Omicron BA.1 variants. We found that the Delta variant binds most strongly to NRP1, while Omicron BA.1 slightly decreases the binding affinity to NRP1 compared to WT, and the van der Waals interaction plays a key role in stabilizing the complexes studied. The change in protonation state of the His amino acid results in different binding free energies between variants. Consistent with the experiment, lowering the pH was shown to increase the binding affinity of the virus to NRP1. Our results indicate that Delta and Omicron mutations not only affect fusogenicity but also affect NRP1 binding.

Presenter: Nguyen Hoang Linh

P.65 – Poster, VCTP-49

Influence of acoustic phonons on nonlinear optical-manegto absorption in special asymmetric hyperbolic quantum wells

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In this work, the nonlinear optical-manegto absorption properties have been theoretically investigated in a special asymmetric hyperbolic quantum well (SAHQW) when electrons are scattered with acoustic phonons (AP). The explicit analytic expression for the magneto-optical absorption coefficient (MOAC) is obtained using the perturbation theory to consider the transition probability for two photon absorption processes. Computational results show that the MOAC as well as the full width at half maximum (FWHM) of the linear and nonlinear optical-manegto resonance peaks both increase with temperature and decrease with the characteristic parameters of the quantum well. Moreover, these results are also compared with different confinement models and with previous studies in both theoretically and experimentally.

Presenter: Lê Đình

P.66 – Poster, VCTP-49

Comparison of entanglement feature, EPR steering, and fidelity of quantum teleportation processes via pair coherent states by photon addition

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In this paper, we investigate and compare the quantum entanglement feature and the EPR steering between the generalized photon-added pair coherent state (GPAPCS) and the superposition photon-added pair coherent state (SPAPCS) by using the Von Neumann entropy criterion and the EPR steering condition. We then use these two states as entanglement resources to quantum teleportation processes, thereby evaluating and comparing the average fidelity of these processes. The results show that both GPAPCS and SPAPCS exhibit high entanglement and steering properties, and have great potential for application in quantum teleportation. Furthermore, in some cases, SPAPCS demonstrates better entanglement and steering properties, and the average fidelity of the quantum teleportation using this state is also higher than that of GPAPCS.

Presenter: Ho Sy Chuong

P.67 – Poster, VCTP-49

Mathematical model describes and analyzes the state of entity σ when entering the time domain P - The application creates new methods for storing and transmitting information data

Tran Dinh An

Ho Chi Minh city University of Technology and Education

The time we perceive in everyday life is a normal concept but there is still no real answer to what is time? It is difficult for us to imagine that our minds and perceptions are placed in a universe with a huge amount of matter and extremely bustling events. This research designs a fictitious but feasible λ closed universe model. In this universe everything seems very simple, there exists only one mathematical entity called the entity σ and there is absolutely nothing else besides this entity. All events occurring in the universe λ are caused by the behavior of entity σ. The signal diagram is a time axis to measure time in λ. When the entity σ exists at a time on the time axis, it is clear that the previous times are all past times of σ in λ and the time domain. This time is called the P time domain. So let's assume entity σ can enter region P on the signal diagram and then analyze how the state of λ will change. According to the butterfly effect, every small impact also creates big changes. The impacts of the entity σ in the P region, whether large or small, also create events that are different from the events that happened in λ, even the fact that σ exists in domain P is an effect. Because those event changes have created a different universe than the original universe, applying the multiverse theory, it can be said that σ entering the P domain means σ entering a parallel universe. But it is still not possible for σ to enter a parallel universe, but research has come up with a method called the λ synchronous method. Because of the special properties of the closed universe system λ and the entity σ, it is entirely possible to create another closed universe system exactly like the original system, then all the events in the original system λ are recreated in the new system λ and adjusted so that events in the new λ begin to occur a period of time later. At this time, let the entity σ jump to the new λ system and one thing has completely happened: the entity σ has entered its own past. When using this method to let σ enter the P region, we can see that the time in the original λ system and the new λ system are events that occur in λ itself, when no events occur, or we can say when the entity σ is at rest, time is also considered to be standing still. Only when σ moves to create events can we feel the existence of what we call "time". So when we gather all our minds and perceptions into such a simple closed system, we can envision two answers to two problems. Firstly, traveling to the past is just going into another parallel universe and wanting to go into another parallel universe is completely feasible but on an extremely small scale and simple until the present times. Second, time can simply be the movements that make up events.

If we consider the entity σ as a bit of information, then the λ synchronous method of bringing σ into domain P can also be used to store and communicate information in a new way. One can imagine how exciting it would be to be able to project bits of information into one's own past and influence to change information that happened before.

Presenter: Trần Đình An

P.68 – Poster, VCTP-49

Investigation of the thermodynamic properties of ABO3 perovskite by the statistical moment method

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We investigate the thermodynamic properties of cubic- structure ABO3 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 ABO3 are also derived. Using the suitable potential with patial charge, the numerical results of the thermodynamic quantities of SrTiO3 and BaTiO3 by the statistical moment method at various temperatures and pressures are obtained. That have shown good agreement with the other theoretical and experimental data. SMM is a great potential to investigate the thermodynamic properties of the various perovskite materials with the cubic structure.

Presenter: Cao Huy Phuong

P.69 – Poster, VCTP-49

Effect of frequency detuning on absorption coefficient in a semiconductor quantum well with a three-levels ladder configuration

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Electromagnetically induced transparency (EIT) is a quantum phenomenon, based on quantum interference, for eliminating the effect of a medium on a propagating beam of electromagnetic radiation. Almost all research on EIT has been studied extensively in atomic vapor systems but have not been studied much in low-dimensional semiconductor materials. In this paper, we study the effect of frequency detuning on absorption coefficient in a semiconductor quantum well with a three levels Ladder-configuration for studying the EIT. We use the density matrix equation for the system under the simultaneous effects of the probe and coupling lasser beams. Using approximate rotational waves and approximate electric dipoles, we obtain the analytical expressions of the absorption coefficient. The results show that in the quantum well with the Ladder-configuration, the absorption spectrum appears a transparent window for the probe laser

beam called EIT window. The depth and width or the position of the EIT window can be altered by frequency detuning of the laser field.

Keywords: semiconductor quantum well, absorption coefficient, electromagnetically induced transparency, frequency detuning.

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Presenter: Tran Cong Phong

P.70 – Poster, VCTP-49

Simulation of neutron and nuclear fragment productions in nucleus-nucleus interactions using the coupling UrQMD 3.4 + SMM model

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The UrQMD model is widely applied for simulation of nucleus-nucleus interactions at high energies. It allows one to generate multi-particle production in the interactions in the so-called

"cascade" mode [1]. We couple the model with the Statistical Multi-fragmentation Model (SMM) to simulate the neutron and nuclear fragment productions using the EoS mode of the UrQMD model. In the coupling mode, the molecular type propagation of nucleons is used accounting potential interactions, stochastic scatterings and multi-particle productions. The evolution time is chosen to equal to 100 fm/c. At the end of the time evolution, the well-known clusterization algorithm is applied for creation of the nuclear pre-fragments in the equal velocity reference frame (clusterization radius Rc = 3 fm). An excitation energy of a pre-fragment is computed as a difference between sums of the kinetic and potential energies of nucleons, and a ground state mass of the pre-fragment. We check that the combination of UrQMD and SMM allows to describe neutron spectra in the reactions – p+Al, Fe, and Pb [2]. Fragment mass distributions in nucleus-nucleus interactions are also analyzed. The combination can be a good candidate to use at NICA and FAIR facilities.

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Presenter: Lê Thị Quỳnh Trang

P.71 – Poster, VCTP-49

Unrevealing the Roles of Defect Species in Absorption and Photo-degradation of Methylene Blue on the Nitrogen-Doped Anatase TiO2 Surface

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The utilization of TiO2 nanostructures for photocatalytic applications has garnered significant attention for more than 60 years. Particularly, nitrogen doping of TiO2 surfaces has demonstrated outstanding performance compared to pristine TiO2 in terms of stability and photocatalytic efficiency. In this study, employing first-principles computational methods and combining the standard semi-local approximation with the highly accurate hybrid functional formalism for the exchange-correlation functional, we investigated the energetic and electronic properties of oxygen vacancy and nitrogen-related defects on the (110) surface, known for its high energetic favorability. We elucidate the functional contributions of these defects to enhanced photocatalysis, which include the reduction of the band gap, defect-mediated photoabsorption, and the decrease in electron-hole pair recombination. Particularly noteworthy is the role of the nitrogen substitution oxygen defect in enhancing Methylene Blue absorption, thus increasing catalytic reactivity. Additionally, we conducted a detailed analysis of the stabilization of these defects in relation to their local structures. This analysis offers theoretical insights into the defects' engineering and their potential applications.

Presenter: Ngoc Linh Nguyen

S.1 – S Poster, VCTP-49

Magnetic Bound State Using Neodymium Magnets

Hoang-Minh Do (1), Van-Duy Nguyen (2)

(1) Hanoi Amsterdam High School for the Gifted, (2) Phenikaa University

This presentation explores the theoretical calculation and realization of a magnetic bound state

using neodymium permanent magnets. Experiments demonstrate that a bound state can be obtained between two free bodies with magnetic dipole moments. The radial stiffness, provided by the static component of a rotating field, is sufficient to support the weight of a floating magnet. This static component is generated by offsetting the dipole center relative to the rotation axis and aligning the dipole with the radial plane. Our study includes the principles, experimental setup, and potential applications of this magnetic bound state.

Presenter: Do Hoang Minh

S.2 – S Poster, VCTP-49

The Dynamics of a Sphere Rolling Upwards on Diverging Inclined Guides

Khanh Hoang Pham Minh (1), Van-Duy Nguyen (2)

(1) Newton Grammar School; (2) Phenikaa University

We propose an analytic and numerical solution to the mechanical paradox of a sphere rolling upwards on two diverging inclined guides. This paradox challenges gravity, as the sphere appears to move uphill. Our approach develops a theoretical framework combining dynamics and energy conservation to explain this phenomenon. We derive and solve the equations governing the sphere's motion analytically and numerically under various conditions.

Presenter: Hoang Pham Minh Khanh

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