Program & Abstracts

48th Vietnam Conference on Theoretical Physics

HỘI NGHỊ VẬT LÝ LÝ THUYẾT VIỆT NAM LẦN THỨ 48

Đà Nẵng

31 July-3 August 2023

Program & Abstracts

48th Vietnam Conference on Theoretical Physics

Mường Thanh Luxury Da Nang Hotel
270 Võ Nguyên Giáp Street
Ngũ Hành Sơn District, Đà Nẵng, Việt Nam

31 July - 3 August, 2023

Contents

Welcome Message

It is a great pleasure to welcome you to the 48th Vietnam Conference on Theoretical Physics (VCTP-48).

The VCTP-48 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.

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 130 participants. 10 invited talks, 17 oral and 66 poster contributions will be presented.

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)

Chair

- Bach Thanh Cong (VNU University of Science, Hanoi)

Organizing Committee

- Tran Minh Tien (Institute of Physics, VAST), Chair
- Trinh Xuan Hoang (Institute of Physics, VAST)
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Secretariat

- Duong Thi Man (Institute of Physics, VAST, Hanoi)

Sponsors

- International Centre of Physics (ICP), Institute of Physics, Vietnam Academy of Science and Technology

General Information

Conference venue

The VCTP-48 conference takes place in:

Mường Thanh Luxury Da Nang Hotel
270 Võ Nguyên Giáp Street,
Đà Nẵng, Việt Nam

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 of the Mường Thanh Luxury Da Nang Hotel. Please follow the direction in the lobby to go to the conference room.

Lunches

Lunches are provided for conference participants in the Mường Thanh Luxury Da Nang 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 participants are invited to the Gala dinner:

Time: 2 August 2023, from 19:00 PM
Place: Mường Thanh Luxury Da Nang Hotel.

For your family members to attend the Gala Dinner, please buy tickets from the conference secretary on 31 July.

VTPS Meeting

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

Time: 17:15 PM - 18:30 PM, Monday, 31 July 2023.
Place: Mường Thanh Luxury Da Nang Hotel.

VTPS Young Research Award

At the opening session of the conference will be an announcement and the delivery of the 2023 VTPS Young Research Award.

Program timetable

Time	Monday, 31 July	Tuesday, 1 August	Wednesday, 2 August	Thursday, 3 August
08:30 – 10:00	Registration (8:30) Opening (9:00) VTPS Young Research Award Nguyen Le Anh (I.1) Photo Session *(Chair: Bach Thanh Cong)*	Poster Session 1 *(Chair: Hoang Anh Tuan)*		Poster Session 2 *(Chair: Nguyen Nhu Dat)*
10:00 – 10:30	Coffee break	Coffee break		Coffee break
10:30 – 12:00	Yoshitada Morikawa (I.2) Nguyen Huy Viet (O.1) Do Ngoc Son (O.2) *(Chair: Vu Ngoc Tuoc)*	Kim Hanchul (I.5) Nguyen Thanh Tien (O.7) Huynh Anh Huy (O.8) *(Chair: Nguyen Huy Viet)*		Le Duc Ninh (I.8) Tran Chien Thang (O.13) Vu Hoa Binh (O.14) *(Chair: Nguyen Quang Hung)*
12:00 – 14:00	Lunch	Lunch	Excursion	Lunch
14:00 – 15:30	Nguyen Quang Hung (I.3) Tran Viet Nhan Hao (O.3) Le Tan Phuc (O.4) *(Chair: Le Duc Ninh)*	Luu Tran Trung (I.6) Phan Thi Ngoc Loan (O.9) Trieu Doan An (O.10) *(Chair: Tran Nguyen Lan)*		Tran Nguyen Lan (I.9) Ho Quoc Duy (O.15) Mineo Hirobumi (O.16) *(Chair: Le Van Hoang)*
15:30 – 16:00	Coffee break **(15:30 – 15:45)**	Coffee break		Coffee break
16:00 – 17:30	**(15:45 – 17:15)** Nguyen The Toan (I.4) Nguyen Duy Vy (O.5) Tran Linh (O.6) *(Chair: Nguyen Hong Quang)*	Khuong Phuong Ong (I.7) Tran Van Quang (O.11) Hoang Trong Dai Duong (O.12) *(Chair: Phan Van Nham)*		Nguyen Truong T. Hieu (I.10) Phan Van Nham (O.17) *(Chair: Tran Minh Tien)*
	VTPS Meeting **(17:15)**		Gala dinner **(19:00)**	Closing

Conference Program

Monday, 31 July 2023

Opening Session
Chair: Bach Thanh Cong, Tran Minh Tien

08:30 - 09:00 Registration

09:00 - 09:10 Opening

09:10 - 09:20 Announcement of 2023 VTPS Young Research Award

09:20 - 10:00 I.1 – Invited
Bound-to-continuum approach for low-energy reactions and its implication in nuclear astrophysics
Nguyen Le Anh (Ho Chi Minh City University of Education)

10:00 - 10:10 Photo Session

10:10 - 10:30 Coffee break

Oral Session: *Condensed Matter Physics*
Chair: Vu Ngoc Tuoc

10:30 - 11:10 I.2 – Invited
Hydrogenation process of CO_2 on metal catalysts studied by combined first-principles and machine learning methods
Yoshitada Morikawa (Osaka University)

11:10 - 11:35 O.1 – Oral
Development of machine learning-assisted semi-empirical model for twisted multi-layer materials
Nguyễn Huy Việt (Institute of Physics, Vietnam Academy of Science and Technology)

11:35 - 12:00 O.2 – Oral
CO_2 capture in MIL-88 series by computational methods
Do Ngoc Son (Ho Chi Minh City University of Technology - VNU-HCM)

12:00 - 14:00 Lunch

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

14:00 - 14:40 I.3 – Invited

A heterogeneous and multilayered model with cylindrical configuration for thermoluminescence dating of ancient architectures: a case study with Oc Eo archaeological site in Vietnam

Nguyen Quang Hung (Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City)

14:40 - 15:05 O.3 – Oral

The role of nuclear decay, collectivity and resonances: toward a new definition of collectivity for neutron-rich unstable nuclei

Tran Viet Nhan Hao (Hue University)

15:05 - 15:30 O.4 – Oral

Effect of bubble structure on the nuclear surface

Le Tan Phuc (Duy Tan University)

15:30 - 15:45 Coffee break

Oral Session: *Soft Matter and Biophysics*
Chair: Nguyen Hong Quang

15:45 - 16:25 I.4 – Invited

Investigating active structures of NLRP3-NACHT protein at atomic scale using computational tools

Nguyen The Toan (University of Science, Vietnam National University)

16:25 - 16:50 O.5 – Oral

High-harmonic frequencies in overhang- and T-shaped microcantilevers

Nguyễn Duy Vỹ (Van Lang University)

16:50 - 17:15 O.6 – Oral

Top-leads from Vietnamese natural products for treatment of diabetes mellitus: molecular docking, steered molecular dynamics study and umbrella sampling

Tran Linh (Institute of Fundamental and Applied Sciences, Duy Tan University)

17:15 - 18:30 VTPS Meeting

Tuesday, 1 August 2023

Poster Session 1
Chair: Hoang Anh Tuan

08:30 - 10:00 P.1 – Poster

The effect of the unparticles at muon-muon colliders in the Randall-Sundrum model

Le Mai Dung (HNUE)

08:30 - 10:00 P.2 – Poster

Effects of vacancy on the electronic properties of zigzag buckling silicene nanoribbons

Ngo Van Chinh (Can Tho University)

08:30 - 10:00 P.3 – Poster

Electron correlations, magnetism and spin-orbit coupling in lattice models based on supercells of honeycomb lattice with single-hole defect

Trần Minh Tiến (Institute of Physics)

08:30 - 10:00 P.4 – Poster

The Optimization aspect of the Variational Quantum Eigensolver

Nguyen Vu Linh (Department of Theoretical Physics, Faculty of Physics and Engineering Physics, affiliated with the University of Science, Ho Chi Minh City)

08:30 - 10:00 P.5 – Poster

SARS-CoV-2 Omicron Sub-variants Bind to Human Cells: Evidence from Molecular Dynamics Simulation

Nguyen Hoang Linh (Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 700000, Vietnam)

08:30 - 10:00 P.6 – Poster

Characterizing polar molecules via odd-even high-order harmonic generations

Nguyen Huynh Kim Ngan (Institute of Fundamental and Applied Sciences, Duy Tan University)

08:30 - 10:00 P.7 – Poster

Quantum magnetocapacitance of monolayer silicene in a magnetic field

Đỗ Mười (Pham Van Dong University)

08:30 - 10:00 P.8 – Poster

Machine-learning approach for discovery of conventional superconductors

Vu Ngoc-Tuoc (Hanoi University of Science and Technology)

08:30 - 10:00 P.9 – Poster

Ionized-impurity limited electron mobility in core-shell cylindrical semiconductor quantum wires

Nguyen Nhu Dat (Duy Tan University)

08:30 - 10:00 P.10 – Poster

Broadband laser-driven creation of entangled state by a nonlinear coupling coupler pumped in two modes

Nguyen Thi Thu Trang (The University of Danang - University of Science and Technology)

08:30 - 10:00 P.11 – Poster

Conductivity near the metal-insulator transitions in the disordered Hubbard model at half-filling

Hoang Anh-Tuan (Institute of Physics - VAST)

08:30 - 10:00 P.12 – Poster

Bilayer Honeycomb Spin Lattice with Competing Ferromagnetic and Antiferromagnetic Interactions in Transverse Field

Bạch Thành Công (Faculty of Physics, VNU University of Science)

08:30 - 10:00 P.13 – Poster

Comparison of entanglement properties and fidelity of quantum teleportation processes via pair coherent states by photon addition

Ho Sy Chuong (Dong Nai University)

08:30 - 10:00 P.14 – Poster

Magnetic field–driven optical properties of a Lambda-like system with a structured continuum

Doan Quoc Khoa (The University of Danang - University of Science and Technology)

08:30 - 10:00 P.15 – Poster

Radioelectric Effect In Semi-parabolic Plus Semi-inverse Squared Quantum Wells in the presence of A strong electromagnetic wave (laser radiation)

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

08:30 - 10:00 P.16 – Poster

The Nonlinear Absorption Of Strong Electromagnetic Waves In Semi-parabolic Plus Semi-inverse Squared Quantum Wells Taking Into Account The Two-Photon Absorption Process

Nguyen Quang Bau (Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam)

08:30 - 10:00 P.17 – Poster

Ordered Phase in the spin-1 Heisenberg model on the anisotropic triangular lattice

Nguyễn Văn Hinh (Trường Đại học Công nghiệp Hà Nội)

08:30 - 10:00 P.18 – Poster

Quantum beat oscillations of excitons confined in spherical sector quantum dots

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

08:30 - 10:00 P.19 – Poster

Enhancement of teleportation average fidelity via photon addition operation

Tran Quang Dat (University of Transport and Communications-Campus in HCM City)

08:30 - 10:00 P.20 – Poster

Photostimulated Nernst effect in compositional superlattice under the influence of confined phonon

Tang Thi Dien (VNU University of science)

08:30 - 10:00 P.21 – Poster

Influence of confined acoustic phonons on the acousto-electric field in doped semiconductor superlattices.
Nguyễn Quyết Thắng (Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam)

08:30 - 10:00 P.22 – Poster
Revisiting the degeneracy in the neutrino oscillation parameters
Nguyễn Thị Hiền (The Institute For Interdisciplinary Research in Science and Education (IFIRSE))

08:30 - 10:00 P.23 – Poster
Quasi–plasmon–polaritons and Higgs mechanism II
Nguyen Van Hoa (HCMUE)

08:30 - 10:00 P.24 – Poster
Microrheology of attractive gels formed by critical Casimir forces
Dang Minh Triet (Can Tho University)

08:30 - 10:00 P.25 – Poster
Effective couplings between two photons and axion in the 3-3-1 model
Vo Van Vien (Tay Nguyen University)

08:30 - 10:00 P.26 – Poster
Electronic and vibrational properties of biphenylene network nanoribbons and superlattices
Nguyen Mai Chung (University of Science and Technology of Hanoi (USTH))

08:30 - 10:00 P.27 – Poster
Investigation of isotopic effects in thermodynamic properties of solid neon
Ho Khac Hieu (Duy Tan University)

08:30 - 10:00 P.28 – Poster
Magnetic properties of the spin-1 J1-J3 Heisenberg model on a triangular lattice
Phạm Thị Thanh Nga (Trường Đại học Thủy lợi)

08:30 - 10:00 P.29 – Poster
Quantitative Bohmian Trajectory Analysis for High Harmonic Generation
Le Van Hoang (Ho Chi Minh City University of Education)

08:30 - 10:00 P.30 – Poster
The effect of neutron excess transition density in the study of (^{3}He,t) isobaric single charge-exchange reactions
Phan Nhut Huan (Institute of Fundamental and Applied Sciences, Duy Tan University)

08:30 - 10:00 P.31 – Poster
Investigate nonsequential triple ionization process of atom by mid-infrared laser pulses

Truong Dang Hoai Thu (Ho Chi Minh city University of Education)

08:30 - 10:00 P.32 – Poster
Improving ligand-ranking of AutoDock Vina by changing the empirical parameters
Phạm Thị Ngọc Hân (Viện kỹ thuật công nghệ cao Nguyễn Tất Thành)

08:30 - 10:00 P.33 – Poster
Quantum steering in a PT-symmetric system of three cavities with a weak interaction between the active and passive cavities
Le Duc Vinh (Tinh Gia 3 high school)

08:30 - 10:00 P.34 – Poster
Thermal-Magnetic Effect on the Energy Spectra of a Hydrogen Atom in a Screened Potential Placed in a Uniform Magnetic Field
Lý Duy Nhất (HCMC University of Education)

08:30 - 10:00 P.35 – Poster
Quasiresonant diffusion of wave packets in one-dimensional disordered mosaic lattices
Nguyen Ba Phi (Department of Basic Sciences, Mientrung University of Civil Engineering)

10:00 - 10:30 Coffee break

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

10:30 - 11:10 I.5 – Invited
Density functional theory calculations on the prototypical low-dimensional charge-density-wave system, In atomic wires on Si(111)
Kim Hanchul (Sookmyung Women's University)

11:10 - 11:35 O.7 – Oral
Structural, electronic, and electronic transport properties of the 1D pentagonal single layer PdSe2 materials: a computational approach
Nguyen Thanh Tien (Can Tho University)

11:35 - 12:00 O.8 – Oral
Molecular dynamics study of silicene nanoribbons under the effect of pressure
Huynh Anh Huy (Can Tho University)

12:00 - 14:00 Lunch

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

14:00 - 14:40 I.6 – Invited
From nonlinear optics to attosecond science: Numerical perspective
Luu Tran Trung (University of Hong Kong)

14:40 - 15:05 O.9 – Oral

Effects of Dynamic Core-Electron Polarization on High-Order Harmonic Generation from Multielectron Molecules
Phan Thi Ngoc Loan (Ho Chi Minh City University of Education)

15:05 - 15:30 O.10 – Oral
Real-time monitoring molecular dynamics using high-order harmonic generation
Trieu Doan-An (Computational Physics Key Laboratory, Department of Physics, Ho Chi Minh University of Education)

15:30 - 16:00 Coffee break

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

16:00 - 16:40 I.7 – Invited
Giant Electric-Field-Induced Strain in perovskite thin Films
Khuong Phuong Ong (Institute of High Performance Computing)

16:40 - 17:05 O.11 – Oral
Electronic band structure and thermoelectric properties of bismuth oxychalcogenides
Tran Van Quang (Faculty of Electronics and Telecommunications, VNU University of Engineering and Technology)

17:05 - 17:30 O.12 – Oral
Machine-Learning-Based Prediction of Material Properties from Energy Spectra of Magnetoexcitons in Monolayer Transition Metal Dichalcogenides
Hoàng Trọng Đại Dương (Ho Chi Minh City University of Education)

Wednesday, 2 August 2023

08:00 - 16:00 Excursion

19:00 - 21:00 Gala dinner

Thursday, 3 August 2023

Poster Session 2
Chair: Nguyen Nhu Dat

08:30 - 10:00 P.36 – Poster
Thermoelectric transport on a weak link between two charge Kondo circuits
Nguyen Hong Quang (Institute of Physics, VAST)

08:30 - 10:00 P.37 – Poster
Analysis of thermodynamic parameters of metallic platinum in anharmonic EXAFS theory under the influence of thermal disorders
Tống Sỹ Tiến (Trường Đại học Phòng cháy chữa cháy)

08:30 - 10:00 P.38 – Poster

Optical Absorption Coefficient and Refractive-Index Change in Weyl semimetal thin films

Huynh V. Phuc (Dong Thap Unversity)

08:30 - 10:00 P.39 – Poster

Polyacrylonitrile-derived porous carbon nanofiber activated by terephthalic acid as free-standing anodes for lithium-ion batteries

Le Dang Manh (Nguyen Tat Thanh University)

08:30 - 10:00 P.40 – Poster

Identifying inhibitors of NSP16-NSP10 of SARS-CoV-2 from large databases

Nguyen Quoc Thai (Dong Thap Unversity)

08:30 - 10:00 P.41 – Poster

Thermodynamic properties of competing magnetic interaction systems in perspective of Monte Carlo simulation and effective field theory

Bach Huong Giang (VNU University of Science)

08:30 - 10:00 P.42 – Poster

Influence of Kerr nonlinearity on electromagnetically induced grating in a three-level lambda-type atomic system

Doai Van Le (Vinh University)

08:30 - 10:00 P.43 – Poster

Dual-channel Optical bistability in a four-level atomic system with a static magnetic field

Luong Thi Yen Nga (Vinh University)

08:30 - 10:00 P.44 – Poster

Double and triple occupancies in large mass imbalance mixtures

Nguyễn Hồng Sơn (Trường Đại học Công đoàn)

08:30 - 10:00 P.45 – Poster

Electron-phonon correlations inducing excitonic excitations in semimetal and semiconducting materials

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

08:30 - 10:00 P.46 – Poster

Excitonic insulator in the mass imbalance extended Falicov–Kimball model

Nguyen Thi Hau (HaNoi University of mining and geology)

08:30 - 10:00 P.47 – Poster

C4N3BN monolayer with persistent half-metallic magnetism

Phạm Nam Phong (Hanoi University of Science and Technology)

08:30 - 10:00 P.48 – Poster

Stationary characteristic quantities of contact interaction particle system in a harmonic trap or an optical lattice at extremely low temperature

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

08:30 - 10:00 P.49 – Poster

Searching for AChE inhibitors from natural compounds by using machine learning and atomistic simulations

Thai Quynh Mai (Ton Duc Thang University)

08:30 - 10:00 P.50 – Poster

Re-investigation of heat capacity in some nuclei

Le Thi Quynh Huong (University of Khanh Hoa)

08:30 - 10:00 P.51 – Poster

Second order of perturbation theory as an analytical description for energy spectra of exciton in monolayer transition-metal dichalcogenides

Dinh Thi Hanh (Ho Chi Minh City University of Education)

08:30 - 10:00 P.52 – Poster

Investigating the Klein tunneling effect through a rectangular potential barrier in binary waveguide arrays

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

08:30 - 10:00 P.53 – Poster

Study of the thermodynamic properties of SrTiO3 perovskite by the statistical moment method

Cao Huy Phuong (Hung Vuong university)

08:30 - 10:00 P.54 – Poster

Dynamical entanglement and quantum teleportation via generalized photon-added pair coherent state under damping effect

Le Thi Hong Thanh (Quang Nam University)

08:30 - 10:00 P.55 – Poster

The enhancement of Pauli blocking effect in odd-nuclei pairing

Tran Vu Dong (University of Science, VNU-HCM)

08:30 - 10:00 P.56 – Poster

Hubbard parameters of Bi2O2Se from linear-response calculation

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

08:30 - 10:00 P.57 – Poster

Impact of screening and relaxation in weakly coupled 2D macromolecular heterostructures: implications for switchable molecular spin-coupling

Rauls Eva (University of Stavanger, Department of Mathematics and Physics)

08:30 - 10:00 P.58 – Poster

An upgrade to Lilith - a tool for constraining new physics from Higgs measurements

Nguyễn Đặng Bảo Nhi (University of Science, VNU-HCM)

08:30 - 10:00 P.59 – Poster

Transmembrane Amyloid β-Peptide Structures: In Silico Study
Ngo Son Tung (Ton Duc Thang University)

08:30 - 10:00 P.60 – Poster
Unlocking the Potential of GeS Monolayer: Strain-Enabled Control of Electronic Transports and Exciton Radiative Lifetimes
Vo Khuong Dien (Researcher)

08:30 - 10:00 P.61 – Poster
Observe muon decay with plastic scintillators, sipm, simplified electronics and data acquisition
Sang Thanh Truong (The Institute For Interdisciplinary Research in Science and Education)

08:30 - 10:00 P.62 – Poster
Effect of temperature on the compressibility in the semiconductor quantum well-wires
Le Van Tan (Van Lang University)

08:30 - 10:00 P.63 – Poster
The reconstruction of divacancies in zigzag-edge buckling silicene nanoribbons
Pham Nguyen Huu Hanh (Can Tho University)

08:30 - 10:00 P.64 – Poster
Thermoelectric transport across a tunnel contact between two charge Kondo circuits
Nguyen Thi Kim Thanh (Institute of Physics, VAST)

08:30 - 10:00 P.65 – Poster
Studying and predicting Energy Gap of materials by Machine Learning Method
Le Huu Nghia (College of Natural Sciences - Can Tho University)

08:30 - 10:00 P.66 – Poster
Thermodynamic properties of hcp structural metals under high pressure
Nguyen Thi Hong (Hong Duc university)

08:30 - 10:00 P.67 – Poster
A DFT investigation of methanal gas absorption on monolayer MS_2 (M=W, Mo)
Tran Quang Huy (Hanoi Pedagogical University 2)

10:00 - 10:30 Coffee break

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

10:30 - 11:10 I.8 – Invited
Multiboson production at the LHC
Le Duc Ninh (Phenikaa University)

11:05 - 11:30 O.13 – Oral

Study of radiative decays $D^*_{(s)} \to D_{(s)}\gamma$
Tran Chien-Thang (Ho Chi Minh City University of Technology and Education)

11:35 - 12:00 O.14 – Oral
New scalar fields in the 3-3-1 model with axion like particle
Vu Hoa Binh (Institude of Physics, VAST)

12:00 - 14:00 Lunch

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

14:00 - 14:40 I.9 – Invited
Development of correlated mean-field theory beyond density functional theory
Tran Nguyen Lan (International University, VNU-HCM)

14:40 - 15:05 O.15 – Oral
Computational Study of the Adsorption of Small Gas Molecules on Pillar[n]arenes
Ho Quoc Duy (Stavanger University)

15:05 - 15:30 O.16 – Oral
Theoretical study of the relation between the dressed states and dynamic Stark shift in presence of non-resonant elliptically polarized laser
Mineo Hirobumi (STAI, Van Lan University)

15:30 - 16:00 Coffee break

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

16:00 - 16:40 I.10 – Invited
2D Wannier-Mott exciton binding energy and diamagnetic shift
Nguyen-Truong T. Hieu (Dong Nai Technology University)

16:40 - 17:05 O.17 – Oral
Magnetic properties in diluted magnetic semiconductors
Phan Van Nham (Duy Tan University)

17:05 - 17:30 Closing

Conference Abstracts

I.1 – Invited, VCTP-48

Bound-to-continuum approach for low-energy reactions and its implication in nuclear astrophysics

Nguyen Le Anh

Department of Physics, Ho Chi Minh City University of Education (HCMUE)

The Skyrme Hartree-Fock framework proves to be a powerful tool for microscopically analyzing low-energy proton-induced reactions, especially in nuclear astrophysics. The cross-sections of proton radiative capture reactions were examined using the bound-to-continuum potential model. Both single-particle bound and scattering states were obtained to calculate the reduced matrix element of the electromagnetic transitions. The low-energy behavior of the astrophysical S factor was extracted. Moreover, the proposed framework can offer a practical approach to explain nuclear scattering at the energies near the proton-emission threshold with minimal experimental input.

Presenter: Nguyen Le Anh

I.2 – Invited, VCTP-48

Hydrogenation process of CO2 on metal catalysts studied by combined first-principles and machine learning methods

Yoshitada Morikawa

Department of Precision Engineering, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

Chemical reactions at surfaces and interfaces play important roles in wide ranges of applications such as heterogeneous catalysis, electrochemistry, fuel cells, batteries, etching processes of semiconductor materials, and so on. In this talk, we will present theoretical investigation and prediction of hydrogenation of CO_2 over Cu catalyst[1,2]. To clarify reaction mechanisms and to identify important factors governing the reactivity of CO_2 on solid surfaces are very important to develop more efficient catalysts or catalytic processes for utilization of CO2. To this end, we investigated CO2 adsorption and hydrogenation[1] on Cu surfaces using van der Waals density functionals as implemented in our home made STATE (Simulation tool for Atom TEchnology) program code [3]. In the second topic, we will discuss the formation process of Cu–Zn surface alloy, which has been extensively involved in the investigation of the true active site of $Cu/ZnO/Al_2O_3$, the industrial catalyst for methanol synthesis which remains under controversy. To provide a better understanding of the dynamic of Cu–Zn surface at the atomic level, the structure and the formation process of the Cu–Zn surface alloy on Cu(997) were inves-

tigated by machine-learning molecular dynamics (MD) [4]. As the third topic, we will discuss the adsorbate-induced surface reconstruction. The adsorbate-induced surface reconstruction might critically determine catalytic activity by altering the morphology of the active sites. We focus on the influence of CO adsorption upon the formation of Cu clusters on the Cu(111) surface [5].

References:

[1] F. Muttaqien, H. Oshima, Y. Hamamoto, K. Inagaki, I. Hamada, and Y. Morikawa, Chem. Comm., 53, 9222 (2017).

[2]. J. Quan, F. Muttaqien, T. Kondo, T. Kozarashi, T. Mogi, T. Imabayashi, Y. Hamamoto, K. Inagaki, I. Hamada, Y. Morikawa, and J. Nakamura, Nature Chemistry, 11, 722-729 (2019).

[3]. Y. Hamamoto, I. Hamada, K. Inagaki, and Y. Morikawa, Phys. Rev. B, 93, 245440 (2016).

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Presenter: Yoshitada Morikawa

I.3 – Invited, VCTP-48

A heterogeneous and multilayered model with cylindrical configuration for thermoluminescence dating of ancient architectures: a case study with Oc Eo archaeological site in Vietnam

Phan Trong Phuc (1), Nguyen Thi Ngoc Hue (1), Pham Thi Hue (1), Tran Tuan Anh (2), Nguyen Khanh Trung Kien (3), Lo Thai Son (1), La Ly Nguyen (1), Tran Dong Xuan (4), Van-Phuc Dinh (5), Nguyen Hoang Long (1), Nguyen Van Tiep (6), Cao Dong Vu (2), Le Ngoc Thiem (7), Ngoc-Quynh Nguyen (7), Hoang Anh Tuan Kiet (8), Luu Anh Tuyen (1), Nguyen Quang Hung (4)

(1) Center for Nuclear Technologies, Vietnam Atomic Energy Institute, Ho Chi Minh City, Viet Nam
(2) Dalat Nuclear Research Institute, Vietnam Atomic Energy Institute, Dalat City, Lam Dong Province, Viet Nam
(3) Southern Institute of Social Sciences, Vietnam Academy of Social Sciences, Ho Chi Minh City, Viet Nam
(4) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City, Viet Nam
(5) Institute of Applied Technology and Sustainable Development, Nguyen Tat Thanh University, Ho Chi Minh City, Viet Nam
(6) Institute of Physics, Vietnam Academy of Science and Technology, Hanoi City, Viet Nam
(7) Institute for Nuclear Science and Technology, Vietnam Atomic Energy Institute, Hanoi City, Viet Nam
(8) Department of Physics & Engineering, West Chester University of PA, West Chester, PA, USA

A heterogeneous and multilayered model with cylindrical configuration has been recently proposed for improving the traditional thermoluminescence dating (TL) technique. Application of the proposed model to four ancient architectures at the Oc Eo – Ba The archaeological site in Vietnam has shown that our model was able to accurately determine the chronologies of architectures having heterogeneous, multilayered and overlapped structures, while conventional spherical and homogeneous model predicted the chronological results of ten to several hundred years higher. Our proposed model also explicitly exhibited the significant contributions of ex-

cavation, destruction, and radiation shielding to the accurate determination of chronology. In particular, with this newly proposed model, we have shown the first scientific evidence for the formation of an overlapped architecture in an architectural assembly at Oc Eo – Ba The, namely there was an (older) architecture constructed around AD 794 and lasted for about 159 years before being destroyed, probably by the kingdom's historical upheavals. Since then, another (younger) architecture was built on top of the older one's foundation [1].

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Presenter: Nguyen Quang Hung

I.4 – Invited, VCTP-48

Investigating active structures of NLRP3-NACHT protein at atomic scale using computational tools

Hien T. T. Lai, Tran-Nam Nguyen, Ha M. Do, Toan T. Nguyen

Key Laboratory for Multiscale Simulation of Complex Systems, and Department of Theoretical Physics, University of Science, Vietnam National University

Since the discovery of the NLRP3 inflammasome by F. Martin and J. Tschopp in 2001 to the present, a large amount of experimental results on cell lines and animal models has shown that NLRP3 has been implicated in many forms of human chronic disease. More specifically, the relationship of NLRP3 activation to the formation and progression of inflammatory diseases such as hepatitis, enteritis, rheumatoid arthritis and gout... At present, NLRP3 is a drug target, however, the understanding of the mechanism of NLRP3 activation, as well as the activators and inhibitors of this process is still unclear. With our previous theoretical work and experimental evidence showing the role of ATP in interacting with and activating the NATCH region of NLRP3, the model is correct. In this study, we continue to use bioinformatics tools, MD with some advantages to evaluate the competitive impact of the interaction between ATP and NACHT of colchicine (named shortly COL) - a compound that has been shown to be effective in diseases associated with NLRP3 such as gout, cardiovascular disease. We docked colchicine to the ATP binding pocket as well as other potential pockets in mouse NACHT model. The best COL configures at pockets with lowest binding scores were chosen underwent molecular dynamics (MD) simulation. Our results show that (i) all systems NACHT-COL are stable after first 20ns simulation time; (ii) COL bind stably to the ATP binding pocket and two other potential pockets of mouse NACHT domain according to high distribution of hydrophobic and van der Waal interactions. While hydrogen bond (Hbond) and electrostatic interactions are important types of contact for keeping ATP at its NACHT pocket; (iii) the compound COL has higher binding energies in other potential pockets than in the ATP pocket. This study provides the activity mechanics of NLRP3 protein and insights into virtual screen phytocompounds with high binding affinity for gout treatments.

Presenter: Nguyen The Toan

I.5 – Invited, VCTP-48

Density functional theory calculations on the prototypical low-dimensional charge-density-wave system, In atomic wires on Si(111)

Hanchul Kim

Department of Materials Physics and Institute of Advanced Materials and Systems, Sookmyung Women's University, Seoul 04310, Korea

Metal-adsorbed semiconductors have attracted much interest in surface science because they provide valuable platforms for studying exotic low-dimensional phenomena. Indium (In) atomic wires self-assembled on the Si(111) surface is a prototypical quasi-one-dimensional (quasi-1D) system undergoing a structural phase transition from the room-temperature (RT) 4×1 to the low-temperature (LT) 8×2 structure at 120K, which is known to be a charge density wave (CDW) condensation. This structural phase transition is known to be accompanied by an electronic metal-insulator transition. This presentation will discuss a comprehensive set of density functional theory calculations for the Si(111)In system. First, the atomic structure of the RT phase and its electronic structure will be discussed. Secondly, the atomic and electronic structures of the LT-8×2 CDW phase will be described in conjunction with the microscopic mechanism of phase transition. Then, I will describe the defect-related phenomena focusing on the effects on the CDW phase transition. Finally, I will deliver an understanding of topological solitons in the LT-8×2 phase. The results from atomic-resolution scanning tunneling microscopy experiments will be frequently introduced throughout the presentation to verify the theoretical predictions.

Presenter: Kim Hanchul

I.6 – Invited, VCTP-48

From nonlinear optics to attosecond science: Numerical perspective

Luu Tran Trung

Department of Physics, The University of Hong Kong

Since the invention of the laser, interaction of light and matter has found a tremendous number of applications. The constant development of intense light sources opened avenues for research in nonlinear optics and extreme nonlinear optics. At the forefront of extreme nonlinear optics is attosecond science, science of phenomena happening in attosecond (1 attosecond = 10^{-18} seconds) timescale. It was developed almost four decades ago and it has been constantly expanded over the years. Nowadays, attosecond science covers researches in all phases of matter: gas, liquid, solid, and plasma. In this talk, we will lead you through a journey, starting from linear physics to nonlinear optics and arriving to attosecond science, all from the numerical perspective. In addition, we will also discuss few notable experiments and the associated results. Last but not least, emerging opportunities for theoretical/numerical investigation in strong field laser physics are discussed.

Presenter: Luu Tran Trung

I.7 – Invited, VCTP-48

Giant Electric-Field-Induced Strain in perovskite thin Films

Khuong Phuong Ong (1), Huajun Liu (2), Kui Yao (2,3) and John Wang (3,4)

(1) Institute of High Performance Computing (IHPC), Agency for Science, Technology and Re-

*search (A*STAR), 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632, Republic of Singapore*
*(2) Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR), 2 Fusionopolis Way, #08-03 Innovis, Singapore 138634, Republic of Singapore*
(3) Department of Materials Science and Engineering, National University of Singapore, Singapore 1175742, Republic of Singapore
(4) NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, Singapore 119077, Republic of Singapore

High-performance sensors and actuators require a large electromechanical response in materials. Normal approach to enhance electromechanical coupling is based on morphotropic phase boundaries requiring stoichiometric control of complex compositions such as in PZT materials. Such mechanism, however, has a drawback on the low Curie temperature. To go beyond this approach, we have proposed [1] a new material structure with nanopillar regions in perovskites oxides thin film $NaNbO_3$. By this, we have achieved a giant piezoelectricity with piezoelectric coefficient, d33= 1098pm/V at 1Khz, and high Curie temperature Tc 4500C. In this talk, we will elucidate the mechanism of high performance piezoelectricity in perovskite $NaNbO_3$.

[1] Huajun Liu, H. Wu, Khuong P. Ong, et al., Science. 369, 292 (2020)

Presenter: Khuong Phuong Ong

I.8 – Invited, VCTP-48

Multiboson production at the LHC

Le Duc Ninh, Dao Thi Nhung

PHENIKAA University, Hanoi, Vietnam

I will review the status of diboson and triboson production processes at the LHC. Anomalous gauge couplings, joint polarization, and related topics will be discussed.

Presenter: Le Duc Ninh

I.9 – Invited, VCTP-48

Development of correlated mean-field theory beyond density functional theory

Lan Nguyen Tran

International University, Vietnam National University – Ho Chi Minh City

I will present our development of a correlated mean-field theory: OBMP2. In our method, an effective Hamiltonian is derived using canonical transformation. Cumulant approximation is then used to reduce the many-body operators into one-body operators. The effective one-body Hamiltonian is diagonalized to update orbitals and orbital energies, resulting in a self-consistency. We have tested our method for molecular systems and found that our method outperforms widely used methods like density functional theory (DFT) and many-body perturbation theories. We also combine our method with a current state-of-the-art quantum computing algorithm, VQE, to simulate challenging molecules. We are also extending our method for materials.

[1] Nhan Trong Le, Lan Nguyen Tran, "Correlated reference-assisted variational quantum eigensolver", J Phys Chem A, 2023 accepted.

[2] Lan Nguyen Tran, "Can second-order perturbation theory accurately predict electron density

of open-shell molecules? The importance of self-consistency", Phys Chem Chem Phys 24 19393, 2022.

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Presenter: Tran Nguyen Lan

I.10 – Invited, VCTP-48

2D Wannier-Mott exciton binding energy and diamagnetic shift

Hieu T. Nguyen-Truong

Dong Nai Technology University

By approximately solving the Schrödinger equation for two-dimensional (2D) Wannier-Mott excitons with and without magnetic fields, we derive expressions for the exciton energy level and the diamagnetic coefficient. We use the approximate Rytova-Keldysh potential to describe the electron-hole interaction, taking into account environmental effects. Our results [1, 2] agree well with experimental data.

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Presenter: Nguyen-Truong T. Hieu

O.1 – Oral, VCTP-48

Development of machine learning-assisted semi-empirical model for twisted multi-layer materials

Huy-Viet Nguyen (1) and Cong-Huy Pham (2)

(1) Institute of Physics, Vietnam Academy of Science and Technology, Hanoi 10072, Vietnam
(2) Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, California 94550, United States

Twisted layer materials have recently attracted much interest due to its fascinating properties, such as the observation of unconventional superconductivity, the flat bands near Fermi energy, leading to strong electronic localization in bilayer graphene at 'magic' twisted angle. From the computational standpoint, it is extremely challenging to perform direct quantum calculations for such systems, due to the large number of atoms in the unit-cell (can be 10-100 thousands or more). As a first step to achieve a viable description of twisted layer materials with the accuracy of first-principles quantum mechanical methods, we develop a machine learning-assisted semi-empirical model for twisted multi-layer graphene. We show that our model, while maintaining the accuracy of density-functional theory calculations, results in orders of magnitude improvement in computational cost. This would allow us to obtain accurate quantum data for very large systems which would not be possible with standard quantum approaches. We compare our calculation for structural properties and electronic band structure to previous published data. Our model also shows good transferability as it can describe reasonably well the structural properties of other carbon polymorphs at ambient conditions.

Presenter: Nguyễn Huy Việt

O.2 – Oral, VCTP-48

CO_2 capture in MIL-88 series by computational methods

Do Ngoc Son

Ho Chi Minh City University of Technology (HCMUT), 268 Ly Thuong Kiet Street, District 10, Ho Chi Minh City, Vietnam. Vietnam National University Ho Chi Minh City, Linh Trung Ward, Ho Chi Minh City, Vietnam. Corresponding author: dnson@hcmut.edu.vn

CO_2 emission has been becoming more and more serious due to the escalation of fossil fuel energy demand. Therefore, CO_2 reduction is an indispensable task to mitigate CO_2 emissions and global warming. MIL-88 series is a promising candidate for CO_2 capture because of its high surface area and large pore size. However, there is no research available to investigate the CO_2 capture capacity in the MIL-88 series and physical insights into their interaction. Therefore, we will discuss the obtained results using computational methods in the present report. Acknowledgement: This research was funded by Vietnam National University Ho Chi Minh City (VNU-HCM) under grant number VL2022-20-01.

Presenter: Do Ngoc Son

O.3 – Oral, VCTP-48

The role of nuclear decay, collectivity and resonances: toward a new definition of collectivity for neutron-rich unstable nuclei

K. Mizuyama (1,2), T. Dieu Thuy (3,4), D. Quang Tam (3,4,5), L. G. Bao Khanh (3,4), T. V. Nhan Hao (3,4)

(1) Institute of Research and Development, Duy Tan University, Da Nang 550000, Vietnam
(2) Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Vietnam
(3) Faculty of Physics, University of Education, Hue University, 34 Le Loi Street, Hue City 52000, Vietnam
(4) Center for Theoretical and Computational Physics, University of Education, Hue University, 34 Le Loi Street, Hue City 52000, Vietnam
(5) Faculty of Basic Sciences, University of Medicine and Pharmacy, Hue University, Hue City 52000, Vietnam

This project is devoted to clarify the relationship between decay, resonance, and collective modes in nuclei. First, we will analyze the nature of the poles of collective modes in the complex plane and classification of resonance types using the Jost-RPA method [1]. Then, the Jost-RPA method will be applied to the nucleon-nucleus scattering in terms of the effect of collective modes and resonances on the absorption effects in nucleon scattering targeting odd nuclei. For nucleon scattering targeting even-even nuclei, the same analysis will be performed using self-consistent PVC [2]. The target nuclei range from stable to neutron-rich nuclei. Based on the results of these analyses, we will also try to give a new definition of collective mode to solve the mystery of collective mode of neutron-rich nuclei.

[1] K. Mizuyama,N. Nhu Le, T. Dieu Thuy, N. Hoang Tung, D. Quang Tam and T. V. Nhan Hao, Phys.Rev.C107,024303(2023).

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Presenter: Tran Viet Nhan Hao

O.4 – Oral, VCTP-48

Effect of bubble structure on the nuclear surface

Le Tan Phuc

Duy Tan University

The depletion of the central density of some nuclei leads to a change in the nuclear surface, specifically the nuclear diffuseness. This comes from the partial nucleon densities which depend on the nuclear single-particle wave function of bubble nuclei. In this report, we analyze the partial density of some bubble nuclei and evaluate their impact on nuclear diffuseness. We also present an ability to study the impact of bubble structure on the reaction rate in nucleosynthesis.

Presenter: Le Tan Phuc

O.5 – Oral, VCTP-48

High-harmonic frequencies in overhang- and T-shaped microcantilevers

Le Tri Dat (1,2), Hong-Hanh Nguyen (3), and Nguyen Duy Vy (4,5)

(1) Computational Laboratory for Advanced Materials and Structures, Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City, Vietnam
(2) Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam
(3) Faculty of Physics and Engineering Physics, University of Science-VNU-HCM, Ho Chi Minh City, Vietnam
(4) Laboratory of Applied Physics, Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Vietnam
(5) Faculty of Applied Technology, School of Technology, Van Lang University, Ho Chi Minh City, Vietnam

letridat@tdtu.edu.vn, nguyenduyvy@vlu.edu.vn

Microcantilever is in the heat of Atomic Force Microscope with versatile functions and applications in vibration transducing, energy harvesting, and highly sensitive measurement. To enhance the measurement sensitivity and bandwidth, several approaches have been exploited on the cantilever structure, such as using multi-mode transduction. For higher-order modes, changing the cross-section is usually used where several holes or cut on the cantilever surface are made. Here, we propose a much simpler structure where the cantilever involves two parts with different widths, the overhang- or T-shaped cantilever. We have shown analytically that the higher-order modes could be tuned to be a multiple of the lower frequency, i.e. the high-harmonic frequencies are obtained. We commented on the potential of using this structure on the real fabrication and application

Presenter: Nguyễn Duy Vỹ

O.6 – Oral, VCTP-48

Top-leads from Vietnamese natural products for treatment of diabetes mellitus: molecular docking, steered molecular dynamics study and umbrella sampling

Nguyen Hoang Linh (1,2), Linh Tran (1,2)*

(1) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City

700000, Vietnam
(2) Faculty of Natural Sciences, Duy Tan University, Da Nang City 550000, Vietnam

Medicinal plants have been known and used as a rich source of therapeutic agents all over the world. It has been known that several natural products are important treatments against diabetes mellitus. Human islet amyloid peptide (hIAPP1–37) aggregation is an early step in diabetes mellitus because hIAPP aggregates in type II diabetics to form oligomers that interfere with beta-cell function, eventually leading to the loss of insulin production. In this study, we have collected 342 compounds derived from Vietnamese natural products and investigated their binding affinity to hIAPP1–37 peptide and their mature tetramer fibril via virtual screening using molecular docking method, steered molecular dynamics and umbrella sampling. The results of potential mean force of the ligands and fibrils obtained from umbrella sampling simulations show that four top binding compounds with the strongest binding affinity are Dracorubin (-8.27 kcal/mol), Amentoflavone (-6.72 kcal/mol), Sarsasapogenin (-5.02 kcal/mol), and Diosgenin (-5.07 kcal/mol).

Presenter: Tran Linh

O.7 – Oral, VCTP-48

Structural, electronic, and electronic transport properties of the 1D pentagonal single layer PdSe2 materials: a computational approach

Nguyen Thanh Tien (1), Phạm Thi Bich Thao (1), Nguyen Hai Dang (1,2), Vo Huu Cau (3) and Vu Hoang Huy (1)

(1) College of Natural Sciences, Can Tho University, Vietnam.
(2) Faculty of Fundamental Science, Nam Can Tho University, Vietnam.
(3) Thanh Khe High School, Da Nang, Vietnam.

Two-dimensional novel pentagonal materials (2Dpenta) have gained a lot of attention being a new class of materials with unique properties that could influence future technologies. In this work, the structural, electronic, and transport properties of the pentagonal one-dimensional derivation (nanotubes, nanoribbons) were systematically investigated. The stability and electronic properties of one-dimensional pentagonal single layer PdSe2 (1D p-PdSe2) with different sizes and under uniaxial small strain are investigated by using density functional theory. The studied structures experience an indirect to direct band gap transition with variation of the band gap as the changed size. In addition, under uniaxial small strain, the survey structures are stable and can still keep the pentagonal ring structure. The electronic band structure and band gap are strongly affected by the uniaxial strain. The evolution of band gap versus the strain as linear. The electron transport properties were investigated by calculating the I-V characterization. The results of this investigation bring a better understanding of the 1D p-PdSe2, opens up potential applications in next generation electronic devices and electromechanical sensors.

Presenter: Nguyen Thanh Tien

O.8 – Oral, VCTP-48

Molecular dynamics study of silicene nanoribbons under the effect of pressure

Huynh Anh Huy (1), Truong Quoc Tuan (2), Ong Kim Le (3,4), Nguyen Truong Long (1)

(1) Department of Physics, School of Education, Can Tho University, Can Tho, Viet Nam
(2) Department of Physics, Faculty of Natural Science., Can Tho University, Can Tho, Viet

Nam
(3) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh, Viet Nam
(4) Faculty of Natural Sciences, Duy Tan University, Da Nang, Viet Nam.

We present molecular dynamics (MD) simulations of the formation of penta- and tetra-silicene nanoribbons from the liquid state under the influence of pressure. The initial models consisted of 6049 Si atoms arranged in a penta structure, with a buckling (Δh) of 1.49 Åand interatomic distances of dmin = 2.23 Åand dmax = 2.36 Å. Initially, we relaxed the initial model at 50 K to achieve an equilibrium state. Subsequently, we heated the model to 3000 K to obtain a liquid state. Following this, we cooled the models down to 2000 K and applied pressure by gradually compressing the model along the x-direction, resulting in a density increase ($\Delta\rho$) of 1.5 g.cm^{-3}. Finally, we cooled the model to 300 K for result analysis. The same process was also applied to the model when studying compression at 1500 K and 1000 K. Throughout the simulations, we maintained a constant melting and cooling rate (γ) of 2 × 1011 K.s^{-1}. Various thermodynamic properties such as total energy, pressure, enthalpy change during compression, as well as structural information including the radial distribution function, number of coordinates, angle, mean squared displacement, and diffraction patterns of atomic configuration were analyzed in detail.

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Presenter: Huynh Anh Huy

O.9 – Oral, VCTP-48

Effects of Dynamic Core-Electron Polarization on High-Order Harmonic Generation from Multielectron Molecules

Ngoc-Loan Phan,1 , Kim-Ngan H. Nguyen, 2, Cam-Tu Le,3, Van-Hoang Le, 1*

1 Department of Physics, Ho Chi Minh City University of Education, Ho Chi Minh City, Vietnam.
2 Duy Tan University, Ho Chi Minh City, Vietnam
3 Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City, Vietnam.

In the past few decades, the nonlinear laser-interaction has attracted unprecedented advances in both experimental and theoretical studies. The simplest model is popularly used, called single-active electron (SAE) approximation, where the core electrons are frozen but not the outermost electron. However, the SAE theory significantly deviates from the experimental observation for atoms and molecules with large polarizability; thus, its validation needs to be reconsidered. The core-electron polarization is, in fact, large in a strong laser field, raising a question about the DCeP role. A recent study on the harmonic process has demonstrated the DCeP effect on the dynamic minimum of HHG from CO molecule [1]; however, a comprehensive investigation of the DCeP impact in different aspects of HHG is still desirable. Our recent studies show that the DCeP strongly affects different characteristics of HHG emitted from CO2 and CO molecules in a linearly polarized laser pulse. Firstly, we indicate that the DCeP can shift and sharpen the structural minima in the HHG from CO2 molecules [2]. Then, we demonstrate the significant DCeP effect on the intensity and shape of HHG from CO molecules at harmonics near the cutoff [3]. Finally, we find out that the DCeP dramatically modifies the even-to-odd ratio, i.e., the ratio between the intensities of the even and the average of the two adjacent odd orders [4,5]. The discrepancy between the two cases of including and neglecting DCeP is

especially large, as much as one order. This strong effect of DCeP makes the simulated even-to-odd ratio nicely matches the available experimental data [6,7]. In Ref. [5], we also find out the DCeP impact on the harmonic phase besides the harmonic intensity found in previous studies [1,3,4]. It is natural to ask whether the DCeP effects on different aspects of HHG have the same origin. This report systematically discusses the physical underlying of DCeP imprints in HHG by considering each step of harmonic generation according to the three-step model. We show that the DCeP effect on HHG not only originates from the ionization and recombination steps but also from the propagation one. The propagation step influences the phase of harmonic bursts whose coherence dramatically impacts harmonic intensity. A further electron trajectories analysis is adopted to detect which step plays an essential role in the DCeP effect on harmonic generation. It is indicated that depending on the laser parameter, the weight of each step is differently contributed to the DCeP effect on HHG.

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Presenter: Phan Thi Ngoc Loan

O.10 – Oral, VCTP-48

Real-time monitoring molecular dynamics using high-order harmonic generation

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

Computational Physics Laboratory K002, Department of Physics, Ho Chi Minh City University of Education, Ho Chi Minh City 72711, Vietnam

Chemical reactions are the result of the coupled dynamics of electrons and nuclei in molecules. Hence, finding methods for monitoring molecular dynamics are required for a comprehensive understanding of chemical reactions [1]. Being pioneered by Zewail, the pump-probe scheme using ultrashort laser pulses has become popular and successful in monitoring molecular nuclear vibration, dissociation, isomerism, and so on [2]. This scheme proposes using a “pump" pulse to excite dynamical processes and a “probe" pulse to generate emission of molecular spectra. By measuring a specific spectrum versus time delay between the pump and probe pulses, molecular dynamics can be extracted from the spectral properties.

In practice, mass spectroscopy, Coulomb explosion, photoelectron spectroscopy, high-order harmonic generation (HHG) are different kinds of spectrum for studying molecular dynamics [2,3]. However, HHG, the laser-induced generation of high-frequency photons, is rarely applied, in spite of its high spatiotemporal resolution. Therefore, in our current project, we aim to use HHG to probe molecular dynamics, particularly the dissociation.

Until now, we have been successful in constructing a procedure for simulating HHG in a dissociative process of hydrogen ion. According to this procedure, we first calculate the molecular adiabatic potential energy surfaces (PES); then, we simulate the molecular dynamics, including

laser-induced excitation and nuclear wavepacket evolution on the PES; finally, we calculate the time-delayed HHG by coherently adding HHG from all molecular adiabatic states. Currently, the procedure is being modified for methyl iodide, whose monitoring dynamics process is more challenging due to the presence of the conical intersection between two dissociative surfaces - a critical problem in molecular dynamics [4]. In this report, our newest results will be shown in detail.

[1] T. R. Nelson et al., "Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials," Chemical Reviews 120, 2215 (2020).

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Presenter: Trieu Doan-An

O.11 – Oral, VCTP-48

Electronic band structure and thermoelectric properties of bismuth oxychalcogenides

Tran Van Quang (1) and Nguyen Huy Viet (2)

(1) Faculty of Electronics and Telecommunications, VNU University of Engineering and Technology, Hanoi, Viet Nam;
(2) Institute of Physics, Vietnam Academy of Science and Technology

Recently, a new class of bismuth oxychalcogenides materials (Bi2O2X, X=S,Se,Te) has attracted a lot of attention due to its potential applications in the fields of (opto-)electronic and thermoelectric devices. First-principles simulations based on density-functional theory (DFT) with standard LDA/GGA approximations of xc-energy not only severely underestimate the bandgap but also lead to a negative bandgap of bismuth oxychacogenides in some cases. Since accurate description of the bandgap is important in determining electronic and thermoelectric properties, advanced functionals should be used to resolve the issue. Recently self-consistently determined onsite U and intersite V interactions have been demonstrated to be effective in dealing with the bandgap problem. In this report, we present the results of calculations using advanced funtionals, namely DFT+U+V and HSE06, and show that the description of excited states of bismuth oxychacogenide can be significantly improved and the semiconducting nature is preserved. Thermoelectric coefficient calculations are also carried out for comparisons between different methods and experiments.

Presenter: Tran Van Quang

O.12 – Oral, VCTP-48

Machine-Learning-Based Prediction of Material Properties from Energy Spectra of Magnetoexcitons in Monolayer Transition Metal Dichalcogenides

Duong-D. Hoang-Trong1, Khang Tran2, Ngoc-Loan Phan1, Duy-Nhat Ly1, and Van-Hoang Le1

1 Ho Chi Minh City University of Education, Ho Chi Minh City, Vietnam

2 New Jersey Institute of Technology, Newark, NJ 07102, USA

Extracting material properties such as the exciton-reduced mass μ and $2D$ static polarizability $\chi 2D$ of monolayer transition metal dichalcogenides (TMDCs) from measured exciton energy spectra is essential because these parameters cannot be retrieved directly from experiments [1, 2]. Recently, a method based on the fitting procedure was proposed to recover μ and $\chi 2D$ from s-state exciton energies of WSe_2 and WS_2 [3]. This method is promising for applying to other monolayer TMDCs; however, a huge amount of data needs to be analyzed. Besides, each TMDC semiconduction material necessitates a unique set of parameters in the fitting procedure while repeating the same process, which is time-consuming and expensive. Nevertheless, recent advanced artificial models with machine learning (ML) capabilities are emerging to help solve similar problems [4]. We report some achievements in applying ML to build a simple model for retrieval of material parameters (μ and $\chi 2D$) of any monolayer TMDC from experimental exciton energies of 1s, 2s, 3s, and 4s states. To do it, we have trained the ML model with more than 300 thousand theoretical data sets of exciton energies calculated by the FORTRAN codes constructed by us previously. A prediction is carried out for WSe_2 with the experimental energy data in Ref. [5]. The results demonstrate a very high accuracy of our ML model. First, the predicted parameters are highly compatible with the currently available data. Second, the theoretical energies calculated by the Keldysh model potential with these material parameters coincide well with the experimental data (with errors less than 1% in most cases). Therefore, the constructed ML model are applicable for more other TMDC materials.

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Presenter: Hoàng Trọng Đại Dương

O.13 – Oral, VCTP-48

Study of radiative decays $D^*_{(s)} \to D_{(s)}\gamma$

Chien-Thang Tran (1), Mikhail A. Ivanov (2), Pietro Santorelli (3), Quang-Chau Vo (4)

(1) Ho Chi Minh City University of Technology and Education;
(2) Joint Institute for Nuclear Research, Dubna, Russia;
(3) University of Naples Federico II & INFN, Naples, Italia;
(4) Ho Chi Minh City University of Science

Radiative decays $D^*_{(s)} \to D_{(s)}\gamma$ are revisited in light of new experimental data from *BABAR* and BESIII collaborations. The radiative couplings $g_{D^*D\gamma}$ encoding nonperturbative QCD effects are calculated in the framework of the covariant confined quark model developed by us. We compare our results with other theoretical studies and experimental data. The couplings (in GeV^{-1}) $g_{D^{*+}D^+\gamma} = -0.45(9)$ and $g_{D^{*0}D^0\gamma} = 1.72(34)$ calculated in our model agree with the experimental data $g_{D^{*+}D^+\gamma} = -0.47(7)$ and $g_{D^{*0}D^0\gamma} = 1.77(16)$. The most interesting case is the

decay $D_s^* \to D_s\gamma$, for which recent predictions of lattice QCD ($\Gamma(D_s^* \to D_s\gamma) = 0.066(26)\,\text{keV}$) and light-cone sum rules at next-to-leading order ($\Gamma(D_s^* \to D_s\gamma) = 2.36^{+1.49}_{-1.41}\,\text{keV}$) disagree. Our calculation yields $\Gamma(D_s^* \to D_s\gamma) = 0.55(22)\,\text{keV}$, which falls somehow between the two mentioned results, but larger than those predicted in other studies using quark models or QCD sum rules.

Presenter: Tran Chien-Thang

O.14 – Oral, VCTP-48

New scalar fields in the 3-3-1 model with axion like particle

V. H. Binh, D. T. Huong, H. N. Long, D. V. Soa

Institude of Physics, VAST

The scalar sector of the 3-3-1 model with axion like particle is studied in detail. In the model under consideration, there are two kinds of scalar fields: the bilepton scalars carrying lepton number two and the ordinary ones without lepton number. We show that there is no mixing among these two kinds of scalar fields. We analyze in detail the CP-odd scalar sector of the model to find the physical fields of the axion like particle and a pseudoscalar with mass in the range 100 GeV to 1 TeV. The results are different from others which have been published before. The CP-even scalar sector of the model is analyzed as well. The results of our analysis of the scalar sector allow to accommodate scalar masses in the 100 GeV-1 TeV region.

Presenter: Vu Hoa Binh

O.15 – Oral, VCTP-48

Computational Study of the Adsorption of Small Gas Molecules on Pillar[n]arenes

Quoc Duy Ho and Eva Rauls

Stavanger University, Norway

The adsorption of small gases (CO_2, N_2, CH_4) by Pillar[5]arenes (P[5]A) was studied using DFT-based methods. Small gases can be adsorbed by P[5]A at the cavity site or at a hydroxyl group. $\pi - \pi$ interactions and weak hydrogen bonds are the major contributors to adsorption at the cavity site and OH groups, respectively. Calculated results also demonstrate the selectivity of CO_2 over N_2 and CH_4 in P[5]A adsorption. The effects of P[n]A cavity sizes (n=4, 5, and 6) on CO_2 adsorption were also studied. Due to charge transfer from the four aromatic rings, CO_2 adsorption at the cavity site has the highest binding energy at P[4]A, while the adsorption at hydroxyl groups has similar binding energies on P[4]A, P[5]A, and P[6]A. The number of CO_2 molecules that can be adsorbed at the cavity site depends on the P[n]A cavity size; the larger the cavity, the more CO_2 molecules can be adsorbed before saturation occurs. P[6]A is the optimal choice for selective CO2 adsorption quantity. The density of state calculations show the physical adsorption of gases in P[n]A. Therefore, if P[n]A is used for gas adsorption, it can be reused after suitable desorption.

Presenter: Ho Quoc Duy

O.16 – Oral, VCTP-48

Theoretical study of the relation between the dressed states and dynamic Stark shift in presence of non-resonant elliptically polarized laser

Mineo H (1), Ho Q.H. (2), Phan N.L. (2), Fujimura Y (3)

(1) Science and Technology Advanced Institute (STAI), Van Lang University
(2) Department of Physics, Ho Chi Minh City University of Education
(3) Department of Chemistry, Graduate School of Science, Tohoku University

Owing to the recent development of laser science and technology, the quantum laser control of ultrafast electron dynamics has been explored actively, and laser-induced π-electron rotations and magnetic fields are expected to establish a principle for the next-generation switching or optoelectronics devices. In the past it was commonly accepted that the coherent π-electron rotation could not be generated in low symmetry aromatic ring molecules, which have no degenerate electronic excited state. Recently we demonstrated that the unidirectional π-electron rotation can be generated even in low symmetry aromatic ring molecules using the two linearly polarized lasers under fixed nuclei [1], and the nuclear vibrational effects are also considered in the adiabatic approximation, where a weak coupling of electron-vibrational interaction is assumed [2]. In this talk we show that a stationary angular momentum is generated even in low-symmetry aromatic ring molecule in the photo-dressed state by introducing the relationship between the Stark shift picture and the dressed state picture. It is found that the dressed states are equivalent to the energy eigen states which are formed by two lasers with same frequencies i.e., elliptically polarized laser, and the difference between two pictures is the initial condition at t=0, that is, in the Stark picture only the ground state is initially populated, on the other hand in the dressed state picture, eigen states which consist of the ground and excited states are initially populated.

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Presenter: Mineo Hirobumi

O.17 – Oral, VCTP-48

Magnetic properties in diluted magnetic semiconductors

Phan Van Nham (1), Nguyen Huu Nha (2)

(1) Institute of Research and Development, Duy Tan University (2) Department of Theoretical Physics, VNUHCM-University of Science

The magnetic properties such as ferromagnetic (FM), antiferromagnetic (AFM) instabilities and especially spin fluctuations in diluted magnetic semiconductors are addressed. In the framework of the dynamical mean-field theory, we have found a set of self-consistent equations determining a single-particle Green's function of itinerant carriers of the Kondo lattice models. The magnetization, static and dynamical spin susceptibility functions and then the spin-relaxation rate are evaluated. Our results realize that once the impurity band is partly filled, the system settles in the FM state in case of low temperatures with sufficiently large magnetic coupling. That magnetic order would be replaced by the AFM state in case the impurity band is completely filled. Results of the dynamical spin susceptibility function address the strong spin fluctuations if the temperature reaches the transition value, especially for the situation of large magnetic coupling between the itinerant carrier spin and localized magnetic moments. In this case, the non-linear behavior of the nuclear spin-lattice relaxation rate versus temperature is found indicating the formation of the magnetic coherent bound state or the magnetic clusters before the magnetic ordered transition happens, the spin dynamical properties in DMS thus have been discussed in more profound.

Presenter: Phan Van Nham

P.1 – Poster, VCTP-48

The effect of the unparticles at muon-muon colliders in the Randall-Sundrum model

Le Mai Dung (1), Dao Thi Le Thuy (1), Le Nhu Thuc (1), Bui Thi Ha Giang (1) and Dang Van Soa (2)

1) Hanoi National University of Education, 136 Xuan Thuy, Dich Vong, Cau Giay, Hanoi, Vietnam;
(2) Faculty of Applied Sciences, University of Economics and Technology for Industries, 456 Nguyen Thi Minh Khai, Vinh Tuy, Hai Ba Trung, Hanoi, Vietnam.

A theoretical attempt is made to present the contribution of the unparticles to the two well-known processes Bhabha and Møller scattering. We concentrate on the lepton processes: $\mu^{\pm} + \mu^{-} \to \mu^{\pm} + \mu^{-}$ in Randall-Sundrum mode under the influence of the unparticles. We evaluate differential cross-sections versus the scattering angle θ, total cross-sections versus the scaling dimension dU and the center-of-mass energy. The reach of energy chosen corresponds to the energy region at CMS. The processes are studied when the incoming and outgoing beams of particles are unpolarized and polarized. We also calculated the number of events, based on the luminosity of the colliders at present or in projection in the future in the previous articles. The numerical results show that as unparticles contribute to all the studied processes, the total cross-sections increase at the high energy with the small scaling dimension. The results subsequently lead to the relevance between theories and experiments in the near future as for the total cross-section in the processes we restricted.

Presenter: Le Mai Dung

P.2 – Poster, VCTP-48

Effects of vacancy on the electronic properties of zigzag buckling silicene nanoribbons

Ngo Van Chinh (1,2), Pham Nguyen Huu Hanh (1,3), Nguyen Thi Kim Quyen (1,4), Vu Thanh Tra (5,6)

(1) School of Graduate, College of Natural Sciences, Can Tho University, 3/2 Street, Ninh Kieu District, Can Tho City, Vietnam;
(2) Ho Thi Ky High School, Ca Mau, Viet Nam;
(3) Thoi Thuan Middle and High School, Can Tho, Viet Nam;
(4) Faculty of Engineering and Technology, Kien Giang University, Kien Giang, Viet Nam;
(5) Department of Physics, School of Education, Can Tho University, Can Tho, Viet Nam;
(6) College of science, department of electrophysics, National Yangming Chiaotung University, Taiwan.

In this work, we aim to investigate the electronic structure of buckling silicene nanoribbons (BSiNRs) under the simultaneous effects of vacancies and external fields by using Tight Binding (TB) calculations. The variation of the electronic properties due to the number and the position of vacancies is investigated extensively. Furthermore, we are particularly interested in the correlation of the energy band structure and reconstruction of each defect type. The results showed that, for single vacancy, structure 5-9 is the most feasible, while for di-vacancy, structure 5-8-5 is the most stable. On the other hand, under the impact of external electric fields, the bandgap

and the band shape are strongly modulated. This confirms the energy gap strongly depends on the magnitude of electric field. This study thus unveils some important conditions for controlling the gap as well as the electronic properties of BSiNRs.

Presenter: Ngo Van Chinh

P.3 – Poster, VCTP-48

Electron correlations, magnetism and spin-orbit coupling in lattice models based on supercells of honeycomb lattice with single-hole defect

Tran Thi Thanh Mai, Vu Thi Kim Oanh, Nguyen Huy Viet, and Tran Minh Tien

Institute of Physics, Vietnam Academy of Science and Technology, Hanoi 10072, Vietnam

Lattice models based on supercells of honeycomb lattice with single-hole defect are studied. The lattice models also include the local Coulomb interaction and the spin-orbit coupling. A two-parameters tight-binding model is used to calculate the band structure and the edge magnetism which appears at the boundary of the hole defects in the lattice. Due to the hole defects a band flatness occurs in the band structure. A competition between band flatness, magnetism and topology is revealed.

Presenter: Trần Minh Tiến

P.4 – Poster, VCTP-48

The Optimization aspect of the Variational Quantum Eigensolver

Nguyen Vu Linh

Department of Theoretical Physics, Faculty of Physics and Engineering Physics, affiliated with the University of Science, Ho Chi Minh City

My research primarily focuses on the Optimization aspect of the Variational Quantum Eigensolver algorithm (VQE), a hybrid quantum-classical algorithm designed to find the ground-state energy of the Hamiltonian. I will examine the various algorithms to update the parameters from the approximation to exact and to the state-of-the-art Quantum Natural Gradient Descent algorithm. The Traversed Ising model, a well-known fermion model, serves as the test model for this research. Most of the results were obtained using Qiskit's simulator on a classical computer.

Presenter: Nguyen Vu Linh

P.5 – Poster, VCTP-48

SARS-CoV-2 Omicron Sub-variants Bind to Human Cells: Evidence from Molecular Dynamics Simulation

Hoang Linh Nguyen (1,2), Nguyen Quoc Thai (3), and Mai Suan Li (4)

(1) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 700000, Vietnam
(2) Faculty of Natural Sciences, Duy Tan University, Danang City 550000, Vietnam
(3) Dong Thap University, 783 Pham Huu Lau Street, Ward 6, Cao Lanh City, Dong Thap, Vietnam
(4) Institute of Physics, Polish Academy of Sciences, al. Lotnikow 32/46, 02-668, Warsaw, Poland

The emergence of the variant of concern Omicron (B.1.1.529) of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) aggravates the COVID-19 pandemic due to its very contagious ability. Studies observed that Omicron binds ACE2 more strongly than Wildtype. The prevalence of Omicron in new COVID-19 cases facilities the emergence of novel lineages with improved receptor binding affinity and immune evasion. To shed light on this open problem, in this work, we investigated the binding free energy of the receptor binding domain of the Omicron lineages BA.2, BA.2.3.20, BA.3, BA4/BA5, BA.2.75, BA.2.75.2, BA.4.6, XBB.1, XBB.1.5, BJ.1, BN.1, BQ.1.1 and CH.1.1 to hACE2 using all-atom molecular dynamics simulation and molecular mechanics Poisson-Boltzmann surface area method. The results show that these lineages have increased binding energy to BA.1 lineage in which BA.2.75 and BA.2.75.2 subvariants bind ACE2 PD more strongly than others. The electrostatic force dominates over van der Waals in the interaction between these two proteins.

Presenter: Nguyen Hoang Linh

P.6 – Poster, VCTP-48

Characterizing polar molecules via odd-even high-order harmonic generations

Kim-Ngan H. Nguyen (1,2), Cam-Tu Le (3,4), Ngoc-Loan Phan (5)

(1) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 71008, Vietnam
(2) Faculty of Natural Sciences, Duy Tan University, Da Nang City 50000, Vietnam
(3) Atomic Molecular and Optical Physics Research Group, Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City 72915, Vietnam
(4) Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City 72915, Vietnam
(5) Computational Physics Key Laboratory K002, Department of Physics, Ho Chi Minh City University of Education, Ho Chi Minh City 72711, Vietnam

High-order harmonic generation (HHG) is a powerful tool for probing the structural and dynamical information of matter. Particularly, HHG has been used to retrieve the HOMO (Highest Occupied Molecule Orbital) [1], probe the internuclear distance in a molecule [2], tracking nuclear and electron dynamics [3]. These studies have clearly confirmed that HHG reflects characteristics of the atomic or molecular targets through their interaction with strong laser field. One of the properties of HHG is its symmetry embodiment. Specifically, with the symmetric laser-target system, such as atoms/symmetric-molecules and linear laser fields, HHG spectra contains only odd harmonic orders. When breaking the symmetry of laser-target system either by using an asymmetry target or asymmetry laser pulse, even orders emerge. Thus, the appearance of the even order in the HHG spectra is the manifestation of the asymmetry of a system. The demonstration of the physical quantities characterizing the asymmetry of polar molecules via the odd-even HHG is essential. Recently, we have numerically and analytically proved that the even-to-odd ratio (i.e. the ratio between the intensity of the even order and two adjacent odd harmonic orders) is a universal quantity that only depends on the polar molecules, and is almost unchanged when varying laser parameters [4]. This statement leads us to the question that whether the harmonic phases can also be a characteristic of the polar-molecular target. Moreover, HHG is a quantity that is measured in the frequency domain. By time-frequency transforms such as Gabor transform, one can retrieve the emission of HHG in the time domain, which can give us the microscopic information of the system. In this way, HHG process can be explained by the interference of attosecond bursts emitted as a train with time. Regarding polar molecules, two adjacent attosecond bursts are distinctive both in amplitude and in phase due to the asymmetry of system [5]. The next question is whether the ratio of intensity and

phase difference of two adjacent bursts can characterize the molecular asymmetry, i.e. whether they are stable with changing the laser parameters. If they are, it implies that these quantities are the intrinsic features of the system. Last but not least, is there any relation between these time-domain and frequency-domain quantities? In this work, we simulate the HHG spectra by numerically solving the time-dependent Schrödinger equation. We indicate that the even-to-odd ratio and the phase difference between two adjacent harmonic orders in HHG spectra are universal quantities that characterize the asymmetry of molecular targets. In the time domain, we also prove that the ratio and the phase difference between two adjacent attosecond bursts are also intrinsic properties and reflect the asymmetry of the system. Moreover, we also point out the relation between the time-domain (attosecond bursts) and the frequency-domain (HHG) quantities.

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Presenter: Nguyen Huynh Kim Ngan

P.7 – Poster, VCTP-48

Quantum magnetocapacitance of monolayer silicene in a magnetic field

Do Muoi

Department of Natural Sciences, Pham Van Dong University

In this word, I present a theoretical study of the quantum magnetocapacitance of spin and valley polarized silicene in an external perpendicular magnetic field. The electronic properties of silicene are differrent from those of well-known graphene due to the strong intrinsic spin orbit interaction and buckled structure of silicene. I show that the presence of both spin orbit interaction and electric field yields for the magnetocapacitance a beating pattern at lown and a level splitting at high magnetic field.

Presenter: Đỗ Mười

P.8 – Poster, VCTP-48

Machine-learning approach for discovery of conventional superconductors

Huan Tran(1) and Tuoc N. Vu (2)

(1)School of Materials Science & Engineering, Georgia Institute of Technology, 771 Ferst Drive NW, Atlanta, Georgia 30332, USA (2)Institute of Engineering Physics, Hanoi University of Science & Technology, 1 Dai Co Viet Road, Hanoi 10000, Vietnam

First-principles computations are the driving force behind numerous discoveries of hydride-based superconductors, mostly at high pressures, during the last decade. Machine learning (ML) approaches can further accelerate future discoveries if their reliability can be improved. The main

challenge of current ML approaches, typically aiming at predicting the critical temperature T_c of a solid from its chemical composition and target pressure, is that the correlations to be learned are deeply hidden, indirect, and uncertain. In this paper, we show that predicting superconductivity at any pressure from the atomic structure is sustainable and reliable. For a demonstration, we curated a diverse data set of 584 atomic structures for which λ and $\omega_l og$, two parameters of the electron-phonon interactions, were computed. We then trained some ML models to predict λ and $\omega_l og$, from which T_c can be computed in a postprocessing manner. The models were validated and used to identify two possible superconductors whose $T_c \sim 10^{\smile}15K$ at zero pressure. Interestingly, these materials have been synthesized and studied in some other contexts. In summary, the proposed ML approach enables a pathway to directly transfer what can be learned from the high-pressure atomic-level details that correlate with high-T_c superconductivity to zero pressure. Going forward, this strategy will be improved to better contribute to the discovery of new superconductors. [https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.7.054805]

Presenter: Vu Ngoc-Tuoc

P.9 – Poster, VCTP-48

Ionized-impurity limited electron mobility in core-shell cylindrical semiconductor quantum wires

Nguyen Nhu Dat

Duy Tan University

Electron mobility limited by scattering from ionized impurities has been theoretically investigated for cylindrical semiconductor quantum wires with core-shell structure. Electron screening and dielectric constant mismatch of the core (ϵ_1) and the shell (ϵ_2) materials were taken into account. The mobility was obtained using the memory function approach. The results show that the remote impurity-limited mobility depends on the location of the impurity sheet in the shell. The closer the impurity sheet is to the wire surface, the higher the electron mobility, which can be up to four times greater. The electron mobility is higher for wires coated with a shell, the dielectric constant of which is greater than the dielectric constant of the core. It has also been shown that electron screening weakens with increasing core radius and coating shell thickness, while the mobility, on the contrary, increases. This is due to the greater rate of fall of the impurity potential than the rate of decrease of the electron screening when changing these wire parameters.

Presenter: Nguyen Nhu Dat

P.10 – Poster, VCTP-48

Broadband laser-driven creation of entangled state by a nonlinear coupling coupler pumped in two modes

Nguyen Thi Thu Trang, Doan Quoc Khoa

The University of Danang - University of Science and Technology, Da Nang, Viet Nam

We investigate a system involving two nonlinear oscillators nonlinearly coupled together. The system is excited by two external classical fields, which are supposed to be decomposed into two components, namely a deterministic element and white noise. By using the nonlinear quantum scissors mechanism, we can show that evolution of the system can be closed within a finite set of Fock states and can be generated maximally entangled states. Specially, we can show that the

maximally entangled states change dramatically in comparison to the case of noise parameter of the laser field is not present. The reasonableness achieved results is affirmed by the comparison to that of previous works.

Presenter: Nguyen Thi Thu Trang

P.11 – Poster, VCTP-48

Conductivity near the metal-insulator transitions in the disordered Hubbard model at half-filling

Hoang Anh Tuan (1), Nguyen Thi Hai Yen (1) and Le Duc Anh (2)

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

In this work, the dc conductivity for half-filled disordered Hubbard model near the Mott- and Anderson metal-insulator transitions is calculated within the typical medium theory. The influence of random potential, on-site Coulomb interaction and temperature on the dc conductivity in the model is investigated. The difference in the conductivity near the Mott- and Anderson metal-insulator transitions is shown and discussed.

Presenter: Hoang Anh-Tuan

P.12 – Poster, VCTP-48

Bilayer Honeycomb Spin Lattice with Competing Ferromagnetic and Antiferromagnetic Interactions in Transverse Field

Niem T. Nguyen(1), Giang H. Bach(1), Oanh T. K. Nguyen(2), Duy Huy Nguyen(1), Hai Phong Nguyen(1), Cong T. Bach(1)

(1) Faculty of Physics, VNU University of Science, 334 Nguyen Trai, Hanoi, Vietnam
(2) Electric Power University, 235 Hoang Quoc Viet, Hanoi, Vietnam

Magnetic properties of 2D materials and related van der Waals heterostructure systems are current interesting problems of science and technology [1]. Some structures like the Ising antiferromagnetic (AF) honeycomb spin CrI3 bilayer show sharp transition to the ferromagnetic (FM) state in a certain out-of-plane magnetic field.This first order magnetization process, which is important for application, is investigated in [2] using the model of two FM honeycomb AA-stacking spin layers coupling with each other by AF interaction in the out- of- plane magnetic field perpendicular to spin planes. The present report studies theoretically the thermodynamics and magnetization process of this bilayer honeycomb spin lattice structure for the transverse field case (the field is parallel to the spin plane) using the transverse Ising model (TIM) and mean field approximation (MFA). Temperature and transverse field dependence of the magnetization are calculated numerically and compared with the experiment for the typical antiferromagnet CrI3.

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Presenter: Bạch Thành Công

P.13 – Poster, VCTP-48

Comparison of entanglement properties and fidelity of quantum teleportation processes via pair coherent states by photon addition

Ho Sy Chuong (1), Truong Minh Duc (2)

(1) Dong Nai University, 09 Le Quy Don, Bien Hoa City, Viet Nam
(2) Department of Physics, University of Education, Hue University, Hue City, Viet Nam

In this paper, we investigate and compare the entanglement properties 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. 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 properties and have great potential for application in quantum teleportation. Furthermore, in some cases, SPAPCS demonstrates better entanglement properties, and the average fidelity of the quantum teleportation using this state is also higher than that of GPAPCS.

Presenter: Ho Sy Chuong

P.14 – Poster, VCTP-48

Magnetic field–driven optical properties of a Lambda-like system with a structured continuum

Doan Quoc Khoa (1), Nguyen Thi Thu Trang (1), Hoang Minh Dong (2)

(1) The University of Danang - University of Science and Technology, Da Nang, Viet Nam;
(2) Ho Chi Minh City University of Food Industry, Ho Chi Minh City, Viet Nam

We suggested the Lambda-like system with two bound degenerated states connected to a continuum state under the external magnetic field. This magnetic field is used to split the ground level into two sublevels by the Zeeman shift and both connection to the continuum state. We show that the electromagnetically induced transparency window can be shifted left or right by changing the sign and magnitude of the magnetic field. Furthermore, the sign and magnitude of the group index can be manipulated simply by changing the sign and magnitude of the magnetic field. It is the advantage to light propagation from the slow to the fast light domain and vice versa.

Presenter: Doan Quoc Khoa

P.15 – Poster, VCTP-48

Radioelectric Effect In Semi-parabolic Plus Semi-inverse Squared Quantum Wells in the presence of A strong electromagnetic wave (laser radiation)

Nguyen Dinh Nam(1),, Nguyen Quang Bau(1),*, Vu Hong Phong(1), Dang Thi Thanh Thuy(1)*

(1) Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam

Radioelectric field in semi-parabolic plus semi-inverse squared quantum wells has been studied in the presence of a linearly polarized electromagnetic wave and a strong electromagnetic wave (laser radiation). By using the quantum kinetic equation for electrons in the case of electrons – optical phonons scattering, the analytical expression for the Radioelectric field is obtained as a function of the frequency, the amplitude of the laser radiation and temperature. Numerical results for a specific GaAs/GaAlAs semi-parabolic plus semi-inverse squared quantum wells is also achieved. The results show that the Radioelectric field has a peak and reaches saturation

as the frequency of the laser radiation increases.

Presenter: Nguyen Dinh Nam

P.16 – Poster, VCTP-48

The Nonlinear Absorption Of Strong Electromagnetic Waves In Semi-parabolic Plus Semi-inverse Squared Quantum Wells Taking Into Account The Two-Photon Absorption Process

Cao Thi Vi Ba (1), Nguyen Quang Bau (1), Tran Anh Tuan (1), Nguyen Dinh Nam (1)**

(1) Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam

General analytic expressions for the nonlinear absorption coefficient (NAC) of strong electromagnetic waves (SEMW) caused by confined electrons in Semi-parabolic Plus Semi-inverse Squared Quantum Wells (SPPSISQW) are obtained by using the quantum kinetic equation (QKE) for electrons in the case of electron-optical phonon scattering. A second-order multiphoton process is included in the result. The dependence of the NAC on the amplitude E_0 and the photon energy $\hbar\Omega$ of an SEMW and the temperature T for a specific GaAs/GaAsAl SPPSISQW is achieved by using a numerical method. The computational results demonstrate that the NAC's dependence on photon energy can be utilized for optically detecting the electric subbands in an SPPSISQW. Furthermore, the obtained results are consistent with prior theoretical and experimental findings.

Presenter: Nguyen Quang Bau

P.17 – Poster, VCTP-48

Ordered Phase in the spin-1 Heisenberg model on the anisotropic triangular lattice

Nguyen Van Hinh (1); Pham Thi Thanh Nga (2) and Nguyen Toan Thang (3)

(1): Hanoi University of Industry, 298 Cau Dien, Bac Tu Liem, Hanoi, Vietnam;
(2): Faculty of Electrical and Electronics Engineering, Thuyloi University, 175 Tay Son, Dong Da, Hanoi, Vietnam;
(3): Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi 11108, Vietnam

We study the effect of fluctuations and spatial anisotropy on the stability of the long-range order of the three-sublattice structure in the spin-1 anisotropic Heisenberg model. The Popov-Fedotov functional integral method and the Luttinger-Tizza process were used to calculate the thermodynamic quantities and determine the ground state. The perturbation expansion of the auxiliary-field around mean-field theory was carried out to investigate the effect of thermal fluctuations on ground state energy and sublattice magnetization. The work is motivated by recent theoretical researches and experimental findings on Ni2+ -based compounds.

Presenter: Nguyễn Văn Hinh

P.18 – Poster, VCTP-48

Quantum beat oscillations of excitons confined in spherical sector quantum dots

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

(1) University of Education, Hue University, 34 Le Loi Street, Hue City, Vietnam
(2) University of Sciences, Hue University, 77 Nguyen Hue Street, Hue City, Vietnam
(3) Hai Ba Trung High School, 14 Le Loi Street, Hue City, Vietnam

In this work, we study the exciton quantum beats in spherical sector quantum dots in a three-level model by the renormalized wavefunction method. The wavefunction expression of the exciton in the non-stationary state and the time-dependent absorption intensity of the exciton under the effect of an intensive pump laser resonating with two exciton levels are also provided. The numerical results show that the exciton absorption intensity takes the form of a damped periodic oscillation in the presence of the pump laser. This is the obvious evidence of the exciton quantum beat behavior that has appeared in the quantum dots. In addition, the amplitude and frequency of the beat depend substantially on the geometric parameters, the quantum dot shape, and the pump laser detuning.

Presenter: Le Thi Dieu Hien

P.19 – Poster, VCTP-48

Enhancement of teleportation average fidelity via photon addition operation

Truong Minh Duc (1), Tran Quang Dat (2)

(1) Department of Physics, University of Education, Hue University, Hue, Viet Nam;
(2) University of Transport and Communications, No. 3 Cau Giay Street, Lang Thuong Ward, Dong Da District, Ha Noi, Viet Nam

As we know, the addition of photons to a two-mode squeezed vacuum state (TMSVS) has been shown to enhance the von Neumann entropy of this state. However, this effect reduces the average fidelity of quantum teleportation over traditional protocols. In this paper, using the linear entropy criterion, we demonstrate that the addition of photons can also enhance the entanglement degree of the TMSVS. When using photon-added TMSVSs as the entanglement resources to teleport a coherent state via a non-canonical protocol, the results show that the average fidelity is enhanced by the photon addition operation. This coefficient increases as the number of photons added to the two-mode increases. In addition, we also show that the average fidelity enhancement can also be achieved by increasing the squeezing parameter of the TMSVS.

Presenter: Tran Quang Dat

P.20 – Poster, VCTP-48

Photostimulated Nernst effect in compositional superlattice under the influence of confined phonon

Nguyen Thu Huong (1), Tang Thi Dien (2,), Nguyen Quang Bau (2,*),Tran Khuong Duy (2), Nguyen Dinh Nam (2), Dao Thanh Hue (2)*

(1) Academy of Air Defense and Air Force, Kim Son, Son Tay, Hanoi, Vietnam
(2) Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam

The photostimulated Nernst effect in compositional superlattice under the influence of confined phonon in two cases electron – acoustic phonon scattering and electron–optical phonon scattering is obtained by using the quantum kinetic equation. The results indicate that the Shubinikov-Dehass oscillations have appeared when examining the effect of magnetic field on the Nernst coefficient (NC) in electron–acoustic phonon scattering. The confined phonons not only make the

magnitude of the Nernst coefficient smaller but also more obvious than the case of unconfined phonons. In addition, for the electron–optical phonon scattering, the magneto-photon resonance condition is also proved, the position of resonance NC's peaks is shifted by confined optical phonons. Besides, the Nernst coefficient is decreased significantly as the temperature increases. Our results in this study show that the Nernst effect in compositional superlattice is different from bulk semiconductors.

Presenter: Tang Thi Dien

P.21 – Poster, VCTP-48

Influence of confined acoustic phonons on the acousto-electric field in doped semiconductor superlattices.

Nguyen Van Nghia (1), Nguyen Quyet Thang (2), Nguyen Quang Bau (2).

Đơn vị trực thuộc: (1) Đại học Thủy Lợi;
(2) Đại học Khoa học tự nhiên - ĐH Quốc gia Hà Nội.

qthang52@gmail.com

By using a quantum kinetic equation for eletron, the expression of the acousto-electric field under the influence of confined acoustic phonoons in doped semiconductor superlattices(DSSL) is obtained. From these expression, the acousto-electric field depend on temperature , acoustic wave frequency , Fermi energy level , doped concentration and quantum number m characterizing the phonons confinement. The rerults are numerically calculated for the GaAs:Be/GaAs:Si DSSL and its have showed that the appearance of phonons confinement makes the acousto-electric field value become difirent than the cases of unconfined phonons.

Presenter: Nguyễn Quyết Thắng

P.22 – Poster, VCTP-48

Revisiting the degeneracy in the neutrino oscillation parameters

Nguyen Thi Hien (1,2), Cao Van Son (2), Phan To Quyen (2,3)

(1) University of Science and Technology of Ha Noi
(2) Institute For Interdisciplinary Research in Science and Education (IFIRSE)
(3) Graduate University of Science and Technology

Neutrino massiveness and leptonic mixing are solely discernible evidence for new physics beyond the Standard Model of elementary particles, as revealed by the well-established quantum mechanical phenomenon known as neutrino oscillation. The neutrino experiment typically measures oscillation probabilities as a function of various parameters, which include three mixing angles, one CP-violation phase, and two mass-squared splittings. The problem is that extracting parameters from probability is not unique and, due to parameter degeneracy, can result in numerous solutions. In this work, we look at the iso-probability curves to revisit the degeneracy among neutrino oscillation parameters. We then derive analytical formulas in order to represent these curves. We also will discuss the application of these analytical findings.

Presenter: Nguyễn Thị Hiền

P.23 – Poster, VCTP-48

Quasi–plasmon–polaritons and Higgs mechanism II

Nguyen Van Hoa 1, and Nguyen Tri Lan 2, and Truong Truong Son 1

1Hochiminh University of Education, 280 An Duong Vuong, D.5, Hochiminh City, Viet Nam
2 Institute of Physics,Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Viet Nam hoanv@hcmue.edu.vn

Building upon Anderson's concept, the previous study explores the notion of the massive exchange boson, a key element of the fundamental electromagnetic force in media, as the upper branch of the quasi–plasmon–polariton phenomenon. By employing analogies between condensed matter and particle theory, as well as the concept of emergence, we delve into the mass problem concerning particles and quasi-particles within the framework of the Higgs mechanism. Expanding upon previous research findings, this article primarily focuses on elucidating the rates of mass transfer pertaining to exchange bosons originating from Higgs particles associated with the electromagnetic, strong, and weak fundamental forces. Explicit mathematical formulations are presented to express these transfer rates, along with predictions regarding certain characteristics of Higgs particles and vacuums.

Presenter: Nguyen Van Hoa

P.24 – Poster, VCTP-48

Microrheology of attractive gels formed by critical Casimir forces

Dang Minh Triet

Can Tho University

We report an experimental study of aging colloidal gels formed by attractive critical Casimir forces. These forces allow us to directly tune the particle interactions with temperature as a control parameter. These experimental results show a stiffening of the network elasticity of the attractive colloidal gels with aging time. We also propose a simple model to interpret the structural origin of colloidal aggregates at the particle level. Our results provide new insights into network elasticity on aging attractive gels.

Presenter: Dang Minh Triet

P.25 – Poster, VCTP-48

Effective couplings between two photons and axion in the 3-3-1 model

Hoang Ngoc Long (1), Vo Van Vien (2), and Vu Hoa Binh (1, 3)

(1) Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi, Vietnam
(2) Tay Nguyen University, Buon Ma Thuot, Dak Lak, Vietnam
(3) Graduate University of Science and Technology, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

The one-loop contribution axion-photon-photon coupling is presented in the framework of the 3-3-1 model, in which the loop diagrams are finite. The decay of axion into two photons is demonstrated. This study shows that it is easy to fulfill dark matter candidate conditions for the axion in the model.

Presenter: Vo Van Vien

P.26 – Poster, VCTP-48

Electronic and vibrational properties of biphenylene network nanoribbons and superlattices

Mai-Chung Nguyen (1), Ngo Quang Minh (1), and Huy-Viet Nguyen (2)

(1) University of Science and Technology of Hanoi, Vietnam Academy of Science and Technology, Hanoi 10072, Vietnam
(2) Institute of Physics, Vietnam Academy of Science and Technology, Hanoi 10072, Vietnam

Recently, the biphenylene network, a two-dimensional carbon allotrope that has been synthesized successfully, has been a subject of interest due to its potential, including thermoelectric applications. In this work, we report the results, based on density-functional calculations, of electronic and vibrational properties of various biphenylene network nanoribbons with different widths and edge terminations. Superlattices formed by graphene and biphenylene network are also studied. The obtained results provide the reference data for the development of effective models that can be used to simulate thermoelectric performance of experimental setups.

Presenter: Nguyen Mai Chung

P.27 – Poster, VCTP-48

Investigation of isotopic effects in thermodynamic properties of solid neon

Ho Khac Hieu (1,2), Nguyen Phuoc The (1,2), Huynh Ngoc Toan (1,2), Dang Thanh Hai (3), and Vu Van Hung (4)

1) Institute of Research and Development, Duy Tan University, 03 Quang Trung, Hai Chau, Da Nang 550000, Viet Nam
2) Faculty of Environmental and Natural Sciences, Duy Tan University, 03 Quang Trung, Hai Chau, Da Nang 550000, Viet Nam
3) Vietnam Education Publishing House, 81 Tran Hung Dao, Hoan Kiem, Hanoi, Viet Nam
4) VNU University of Education, 144 Xuan Thuy, Cau Giay, Hanoi 123105, Viet Nam

Isotopic effects in mean-square displacement, specific heat at constant pressure and linear thermal expansion coefficient of solid neon have been considered using the statistical moment method in statistical mechanics. This approach allows us to study these effects including the anharmonicity of lattice vibrations. We implement calculations for ^{20}Ne and ^{22}Ne isotopes in temperature range from 0 K to the melting temperature (24.6 K) using Lennard-Jones potential to describe the interaction between Ne quantum particles. Our numerical results are compared with those of path-integral Monte Carlo simulations and previous experimental data showing the good agreement. This research presents an effective statistical approach to study isotope effects on thermodynamic quantities of materials.

Presenter: Ho Khac Hieu

P.28 – Poster, VCTP-48

Magnetic properties of the spin-1 J1-J3 Heisenberg model on a triangular lattice

Nguyen Van Hinh (1), Pham Thi Thanh Nga (2) and Nguyen Toan Thang (3)

(1) Hanoi University of Industry, 298 Cau Dien, Bac Tu Liem, Hanoi, Vietnam;
(2) Faculty of Electrical and Electronics Engineering, Thuyloi University, 175 Tay Son, Dong Da, Hanoi, Vietnam;
(3) Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh,

Hanoi, Vietnam

We study the spin-1 J1-J3 Heisenberg model with antiferromagnetic nearest neighbors J1>0 and the ferromagnetic third neighbor J3 <0 for a triangular lattice. The ground-state and thermodynamic properties are evaluated from the Popov-Fedotov functional integral method and the Luttinger-Tisza procedure. Perturbation expansion of the auxiliary field around mean-field theory was carried out to investigate the effect of thermal fluctuations on ground state energy and sublattice magnetization. The results are compared with those of the spin wave approximation and experimental data on the compound NiGa2S4.

Presenter: Phạm Thị Thanh Nga

P.29 – Poster, VCTP-48

Quantitative Bohmian Trajectory Analysis for High Harmonic Generation

Cam-Tu Le (1), Ngoc-Loan Phan (2), and Van-Hoang Le (2)

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

Quantitative analysis for high harmonic generation (HHG) based on the quantum trajectory perspective is suggested for CO molecules. We show that the central Bohmian trajectories define the right structure of high harmonic spectra while others, including the outermost trajectories, contribute nonlocally to the HHG intensity. This technique based on counting the number of returning events differs from the three-step model and is useful for explaining the multi-electron effects such as the dynamic core-electron polarization.

Presenter: Le Van Hoang

P.30 – Poster, VCTP-48

The effect of neutron excess transition density in the study of (^{3}He,t) isobaric single charge-exchange reactions

Phan Nhut Huan

Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City, Vietnam

The isobaric single charge-exchange reactions, which are determined directly by the Fermi transition between the isobaric analog state (IAS) and the ground state of the target, can be used to investigate the neutron skin thickness in heavy nucleus. In this study, we analyze the (^{3}He,t)IAS reactions within the framework of Lane model. To determine the microscopic nucleus-nucleus optical potential, we employ the double-folding model using the Argonne v18 G-matrix interaction derived from Brueckner–Hartree–Fock calculation in nuclear matter. The transition potential is determined by considering the isovector and neutron excess density, which are obtained from the Skyrme-Hartree-Fock calculation. The results indicate that a clear improvement in the theoretical prediction of (^{3}He,t)IAS reactions is found when the neutron excess density is used to determine the transition densities. The relation between the neutron skin thickness, and the core-polarization by the Coulomb effect in the description of the (^{3}He,t)IAS reactions is discussed in this work.

Presenter: Phan Nhut Huan

P.31 – Poster, VCTP-48

Investigate nonsequential triple ionization process of atom by mid-infrared laser pulses

Thu D.H. Truong (1,2,3), Hieu V. Tran (3), Hanh H. Nguyen (1,2), Hanh T. Tran (1,2), Vinh N.T. Pham (3,4)

(1) Department of Theoretical Physics, University of Science, Ho Chi Minh City 700000, Viet Nam
(2) Vietnam National University, Ho Chi Minh City 700000, Viet Nam
(3) Department of Physics, Ho Chi Minh City University of Education, Ho Chi Minh City, Viet Nam
(4) Office of Postgraduate Studies, Ho Chi Minh City University of Education, Ho Chi Minh City, Viet Nam

In this study, we use the full classical ensemble model to enhance the calculation process for investigating the momentum distribution of ions in the nonsequential triple ionization (NSTI) of neon atoms driven by mid-infrared laser pulses. The results indicate that our calculation is consistent with previous theoretical and experimental studies of NSTI. In addition, we conclude that the shape of the momentum distribution of Ne^{3+} ions depends on the wavelength and intensity of the laser pulse.

Presenter: Truong Dang Hoai Thu

P.32 – Poster, VCTP-48

Improving ligand-ranking of AutoDock Vina by changing the empirical parameters

T. Ngoc Han Pham (1), Trung Hai Nguyen (2,3), Nguyen Minh Tam (3,4), Thien Y. Vu (1), Nhat Truong Pham (5), Nguyen Truong Huy (1), Binh Khanh Mai (6), Nguyen Thanh Tung (7,8), Minh Quan Pham (8,9), Van V. Vu (10), Son Tung Ngo (2,3)

(1) Faculty of Pharmacy, Ton Duc Thang University, Ho Chi Minh City, Vietnam
(2) Laboratory of Theoretical and Computational Biophysics, Ton Duc Thang University, Ho Chi Minh City, Vietnam
(3) Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam
(4) Computational Chemistry Research Group, Ton Duc Thang University, Ho Chi Minh City, Vietnam
(5) Faculty of Electrical and Electronics Engineering, Ton Duc Thang University, Ho Chi Minh City, Vietnam
(6) Department of Chemistry, University of Pittsburgh, Pittsburgh, Pennsylvania, USA
(7) Institute of Materials Science, Vietnam Academy of Science and Technology, Hanoi, Vietnam
(8) Graduate University of Science and Technology, Vietnam Academy of Science and Technology, Hanoi, Vietnam
(9) Institute of Natural Products Chemistry, Vietnam Academy of Science and Technology, Hanoi, Vietnam
(10) NTT Hi-Tech Institute, Nguyen Tat Thanh University, Ho Chi Minh City, Vietnam

AutoDock Vina (Vina) achieved a very high docking-success rate, p, but give a rather low correlation coefficient, R, for binding affinity with respect to experiments. This low correlation can be an obstacle for ranking of ligand-binding affinity, which is the main objective of docking

simulations. In this context, we evaluated the dependence of Vina R coefficient upon its empirical parameters. R is affected more by changing the gauss2 and rotation than other terms. The docking-success rate p is sensitive to the alterations of the gauss1, gauss2, repulsion, and hydrogen bond parameters. Based on our benchmarks, the parameter set1 has been suggested to be the most optimal. The testing study over 800 complexes indicated that the modified Vina provided higher correlation with experiment Rset1= 0.556±0.025 compared with RDefault = 0.493±0.028 obtained by the original Vina and RVina 1.2 = 0.503 ± 0.029 by Vina version 1.2. Besides, the modified Vina can be also applied more widely, giving R $\geq$ 0.500 for 32/48 targets, compared with the default package, giving R $\geq$ 0.500 for 31/48 targets. In addition, validation calculations for 1036 complexes obtained from version 2019 of PDBbind refined structures showed that the set1 of parameters gave higher correlation coefficient (Rset1 = 0.617±0.017) than the default package (RDefault =0.543±0.020) and Vina version 1.2 (RVina 1.2 = 0.540± 0.020). The version of Vina with set1 of parameters can be downloaded at https://github.com/sontungngo/mvina. The outcomes would enhance the ranking of ligand-binding affinity using Autodock Vina.

Presenter: Phạm Thị Ngọc Hân

P.33 – Poster, VCTP-48

Quantum steering in a PT-symmetric system of three cavities with a weak interaction between the active and passive cavities

Le Duc Vinh (1), Doan Quoc Khoa (2)

(1) Tinh Gia 3 high school, Nghi Son District, Thanh Hoa Province, Vietnam;
(2) University of Science and Technology - The University of Da Nang, Vietnam

A system of three cavities connected by nonlinear couplings is considered in which the coupling between the active and passive cavities is much weaker than the others. We show the dependence of the phase transition point of PT-symmetry on parameters characterizing our system. The generation of quantum steering is also investigated by using steering parameter calculations that show the steering ability of subsystems. We show that in the unbroken phase of PT-symmetry, quantum steering between pairs of subsystems can be one-way or two-way steering depending on the gain and loss of energy in the active and passive cavities. We also point out that the steering abilities of subsystems in our system are strongly dependent on the initial states of the system which are set up with one photon in the active cavity or the passive one.

Presenter: Le Duc Vinh

P.34 – Poster, VCTP-48

Thermal-Magnetic Effect on the Energy Spectra of a Hydrogen Atom in a Screened Potential Placed in a Uniform Magnetic Field

Duy-Nhat Ly (1), Thanh-Truc N. Huynh (2), Duy-Kien Pham (1), Thu-Ha N. Luong (1), Huong-Giang T. Nguyen (1), Huu-Duc Le (1), Van-Hoang Le (1)

(1) Ho Chi Minh City University of Education;
(2) Marie Curie High School, Q3

The energy spectra of a hydrogen atom in a screened potential placed in a uniform magnetic field have been a topic of great interest in plasma physics [1], [2]. Currently, it is possible to create plasma in the laboratory with temperatures reaching several MeV [3]. Consequently, in addition to studying the influence of the magnetic field on the energy spectra of hydrogen atoms,

it is necessary to investigate the thermal movement of the electron-nucleus center of mass in the magnetic field. This effect is taken into account by incorporating the term $-\frac{e}{M}(\mathbf{B}\times\mathbf{K})\cdot\mathbf{r}$ in the exact Hamiltonian, which separates it from the movement of the center of mass [4], [5]. Here, $\mathbf{K}$ represents the pseudo-momentum vector of the center of mass, which is temperature-dependent according to the Maxwell–Boltzmann distribution, given by $\overline{K^2} = 3M\,k_BT$. In this study, we investigate the simultaneous effects of the thermal motion of the center of mass and the magnetic field on the energy spectra, referred to as the thermal-magnetic effect. Perturbation theory is employed to examine this effect while considering the combined influences of temperature and magnetic field on the spectra. Preliminary results indicate that in the ground state, the energy shift is only 0.01 at a temperature of $T = 60\times10^6$K and a magnetic field of $B = 2.35\times10^4$Tesla. Although the influence is small in the ground state, we anticipate a significant thermo-magnetic effect on the energy levels of excited states.

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Presenter: Lý Duy Nhất

P.35 – Poster, VCTP-48

Quasiresonant diffusion of wave packets in one-dimensional disordered mosaic lattices

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

(1) Department of Basic Sciences, Mientrung University of Civil Engineering, Vietnam and Research Institute for Basic Sciences, Ajou University, Korea;
(2) Computing Fundamentals Department, FPT University, Vietnam;
(3) Department of Physics, Ajou University, Korea and School of Physics, Korea Institute for Advanced Study, Korea

We investigate numerically the time evolution of wave packets incident on one-dimensional semi-infinite lattices with mosaic modulated random on-site potentials, which are characterized by the integer-valued modulation period κ and the disorder strength W [1]. For Gaussian wave packets with the central energy E_0 and a small spectral width, we perform extensive numerical calculations of the disorder-averaged time-dependent reflectance, $\langle R(t)\rangle$, for various values of E_0, κ, and W. We find that the long-time behavior of $\langle R(t)\rangle$ obeys a power law of the form $t^{-\gamma}$ in all cases. In the presence of the mosaic modulation, γ is equal to 2 for almost all values of E_0, implying the onset of the Anderson localization, while at a finite number of discrete values of E_0 dependent on κ, γ approaches 3/2, implying the onset of the classical diffusion. This phenomenon is independent of the disorder strength and arises in a quasiresonant manner such that γ varies rapidly from 3/2 to 2 in a narrow energy range as E_0 varies away from the quasiresonance values. We deduce a simple analytical formula for the quasiresonance energies and provide an explanation of the delocalization phenomenon based on the interplay between randomness and

band structure and the node structure of the wave functions. We explore the nature of the states at the quasiresonance energies using a finite-size scaling analysis of the average participation ratio and find that the states are neither extended nor exponentially localized, but critical states.

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Presenter: Nguyen Ba Phi

P.36 – Poster, VCTP-48

Thermoelectric transport on a weak link between two charge Kondo circuits

T. H. Do (1), T. B. Cao (2), T. K. T. Nguyen (2), H.Q. Nguyen (2), M. N. Kiselev (3)

(1) Nguyen Viet Xuan high school, Dai-Dong, Vinh-Tuong, Vinh-Phuc, Vietnam
(2) Institute of Physics, Vietnam Academy of Science and Technology , 10 Dao Tan, Cong-Vi, Ba-Dinh, Hanoi, Vietnam
(3) The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, I-34151, Trieste, Italy

We revisited the setup which has been proposed in Phys. Rev. B 97, 085403 (2018). The generalization of the ideas of Flensberg-Matveev-Furusaki theory is adopted to describe a Integer Quantum Hall charge Kondo circuit. The design of a weak link between two charge Kondo circuits can be a weak coupling between the Fermi and non-Fermi liquid states. We compute the thermoelectric coefficients in the perturbation theory assuming smallness of the reflection amplitudes of the quantum point contacts. The oscillations of the thermoelectric coefficients as functions of the gate voltage of each quantum dot are analyzed in three different scenarios as: Fermi liquid vs Fermi liquid, Fermi liquid vs non-Fermi liquid, non-Fermi liquid vs non-Fermi liquid. Although the Fermi liquid behavior is more prominent than the non-Fermi liquid one, we can find possible experimental realizations of the model to observe the signatures of the non-Fermi liquid behavior in the thermoelectric transport measurements.

Presenter: Nguyen Hong Quang

P.37 – Poster, VCTP-48

Analysis of thermodynamic parameters of metallic platinum in anharmonic EXAFS theory under the influence of thermal disorders

Tong Sy Tien (1,), Nguyen Thi Minh Thuy (1), Vu Thi Kim Lien (1), Ho Van Yen (2), Nguyen Cong Toan (3), Nguyen Bao Trung (3)*

(1) Faculty of Fundamental Sciences, University of Fire Prevention & Fighting, 243 Khuat Duy Tien, Hanoi 120602, Vietnam;
(2) Faculty of Fundamental Sciences, Artillery Officer School, Thanh My, Son Tay, Hanoi 154210, Vietnam;
(3) Department of Physics, Hanoi University of Science, 334 Nguyen Trai, Hanoi 120034, Vietnam

The thermodynamic parameters of metallic platinum (Pt) have been calculated and analyzed under the influence of thermal disorders in the anharmonic Expanded X-ray absorption fine structure (EXAFS) theory. The calculation model is developed based on the correlated Einstein model and quantum-statistical perturbation theory using an effective potential method. Thermodynamic parameters are considered, including the local force constants, Einstein frequency,

Einstein temperature, interatomic distances, mean square relative displacement, and thermal expansion coefficient. The influence of thermal disorders on these parameters is derived from the thermal vibrations of all atoms, with each thermal vibration that is quantized and treated as a phonon, and the anharmonicity is the result of phonon-phonon interactions. The obtained expressions can satisfy all their temperature-dependent fundamental properties. The numerical results of Pt agree well with those obtained from the other theoretical models and experimental data at various temperatures in the range from 0 K to 1000 K. The obtained results indicate that the present model can efficiently investigate the thermodynamic parameters of Pt.

Presenter: Tống Sỹ Tiến

P.38 – Poster, VCTP-48

Optical Absorption Coefficient and Refractive-Index Change in Weyl semimetal thin films

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

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

We theoretically study the optical properties of thin films of Weyl semimetals (WSMs) in the presence of a non-uniform magnetic field. Analytical expressions for the optical absorption coefficients (OACs) and refractive index changes (RICs) are derived using the equation of motion method. The OACs and RICs are evaluated as a function of photon energy for both undoped and doped WSM thin films, considering different values of electron densities, temperatures, and magnetic fields. The electron density plays a significant role in determining the threshold energy in the doped regime. Furthermore, the contribution of right-polarized light to the susceptibilities is consistently dominant compared to the left-polarized light.

Presenter: Huynh V. Phuc

P.39 – Poster, VCTP-48

Polyacrylonitrile-derived porous carbon nanofiber activated by terephthalic acid as free-standing anodes for lithium-ion batteries

Manh Dang Le (1), Loi Tuan Nguyen(2), Phuong Hoai Pham(1), Duy The Nguyen(1), Hieu Trung Bui(1)

(1)NTT Hi-Tech Institute, Nguyen Tat Thanh University, Ho Chi Minh City 700000, Vietnam; (2)Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 700000, Vietnam

This study focuses on the development of porous carbon nanofibers (PCNFs) by electrospinning through the sublimation of terephthalic (PTA) acid for free-standing anodes in lithium-ion batteries. Electrospun fiber mats prepared using polyacrylonitrile (PAN)/PTA in N, N-dimethylformamide solution were carbonized at 900oC for 2 h under vacuum to PCNFs. The free-standing, perforated features PCNFs can be directly applied as an anode in LIBs just after drying without requiring additional conducting additives or polymeric binders. The electrode was characterized using scanning electron microscopy (SEM), surface area analysis (BET), X-ray diffraction (XRD), transmission electron microscopy (TEM), Fourier transform infrared (FTIR), and Raman spectra (Raman). The blending of PTA with PAN resulted in the formation of in-

terconnected pores along the CNFs without changing the diameter. This strategy makes the PCNFs have a surface area of up to 290 m2 g-1 which is significantly higher than the carbon nanofibers (CNFs) with 107 m2 g-1. As a result, electrochemical tests exhibited that the PCNFs have a high discharge capacity of 750 mAh g-1, which is much higher than that of the CNFs (240 mAh g-1) at 100 mA g-1. Even when cycled at 3 A g-1, the PCNFs still exhibit a very high capacity of 621 mAh g-1. These results suggest that PCNFs anodes showed much improved electrochemical performance in comparison to the CNFs in terms of storage capacity, enhanced charge-discharge kinetics, and cycle stability.

Presenter: Le Dang Manh

P.40 – Poster, VCTP-48

Identifying inhibitors of NSP16-NSP10 of SARS-CoV-2 from large databases

Nguyen Quoc Thai (1), Hoang Linh Nguyen (2), Mai Suan Li (3)

(1) Dong Thap University, Cao Lanh 870000, Vietnam
(2) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 700000, Vietnam
(3) Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

The COVID-19 pandemic, which has already claimed millions of lives, continues to pose a serious threat to human health, requiring the development of new effective drugs. Non-structural proteins of SARS-CoV-2 play an important role in viral replication and infection. Among them, NSP16 (non-structured protein 16) and its cofactor NSP10 (non-structured protein 10) perform C2'-O methylation at the 5' end of the viral RNA, which promotes efficient virus replication. Therefore, the NSP16-NSP10 complex becomes an attractive target for drug development. Using a multi-step virtual screening protocol which includes Lipinski's rule, docking, steered molecular dynamics and umbrella sampling, we searched for potential inhibitors from the PubChem and anti-HIV databases. It has been shown that CID 135566620 compound from PubChem is the best candidate with an inhibition constant in the sub-μM range. The Van der Waals interaction was found to be more important than the electrostatic interaction in the binding affinity of this compound to NSP16-NSP10. Further in vitro and in vivo studies are needed to test the activity of the identified compound against COVID-19.

Presenter: Nguyen Quoc Thai

P.41 – Poster, VCTP-48

Thermodynamic properties of competing magnetic interaction systems in perspective of Monte Carlo simulation and effective field theory

*Oanh K.T. Nguyen (2), Phong H. Nguyen (1), Quan M. Le (1), Huy D. Nguyen (1), Niem T. Nguyen (1), Cong T. Bach (1), and Giang H. Bach (1)**

(1) Faculty of Physics, VNU University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam;
(2) Electric Power University, 235 Hoang Quoc Viet, Hanoi, Vietnam

The competition between magnetic interactions such as ferromagnetic (FM) and anti-ferromagnetic (FM) interactions normally occurring in perovskites was employed by a disorder Ising model. By adjusting the probabilities of ferromagnetic (FM) and antiferromagnetic (AFM) interactions, denoted as p and (1-p) respectively, and their magnitudes, we examine magnetic phase transi-

tions by determining the thermodynamic behaviors, for example, magnetization, total energy, spin susceptibility, and specific heat, by using an effective field theory and Monte Carlo simulation. The calculations show that a ferromagnetic to paramagnetic (FM-PM) phase transition is consistently revealed at a critical temperature T_{c2}. However, for certain AFM probability values, another antiferromagnetic to ferromagnetic (AFM-FM) phase transition may occur at lower critical temperatures T_{c1}. While Monte Carlo simulations are advantageous for examining thermodynamic properties at finite temperatures, both with and without an external field, analytical calculations excel particularly in a wide range of temperatures without a field.

Presenter: Bach Huong Giang

P.42 – Poster, VCTP-48

Influence of Kerr nonlinearity on electromagnetically induced grating in a three-level lambda-type atomic system

Le Van Doai, Luong Thi Yen Nga and Ho Hai Quang

Vinh University, 182 Le Duan Street, Vinh City, Vietnam

Diffraction grating is commonly used as dispersive elements in many optical systems for applications including spectrometers, switching, tuning and trimming elements in dense wavelength-division multiplexing, visual display technology, external cavity lasers, etc., [1]. The diffraction efficiency of grating is an important parameter since it will strongly influence the final energy delivered by the optical diffraction system. The coherent interaction between the laser fields with the atom can lead to quantum interference of transition probabilities within the atomic system. The consequence of this quantum interference is to suppress (destructive interference) or enhance (constructive interference) the total transition probability and thus radically change the absorption or transmission property of the atomic medium for a light field. The constructive interference of transition probabilities generates electromagnetically induced transparency (EIT) [2]. Under the EIT condition, the medium forms peculiar optical properties and thus it offers unusual applications such as [3] giant nonlinearity, low threshold optical bistability, and so on. Currently, based on the EIT effect, an atom sample can behave like a diffraction grating which is called an electromagnetically induced grating (EIG) [4]. EIG was first proposed in 1998 [4] and experimentally verified in 1999 [5]. Since then, theoretical and experimental studies of EIG have attracted great attentions [6-10] due to their potential applications in many fields, such as atoms velocimetry [11], light storage [12], beam splitting and fanning [13], shaping a biphoton spectrum [14], controlling multi-wave mixing processes [15], angular Talbot effect [16] and giant Goos–Hänchen shifts [17]. Recently, EIG efficiency has been greatly improved in different atomic systems with the support of other external fields such as microwave field [18] and magnetic field [19], Kerr nonlinearity [20]. In this work, we study the influence of giant Kerr nonlinearity on diffraction pattern of EIG in a three-level lambda-type atomic system. It shows that the efficiency of EIG is significantly improved in the presence of Kerr nonlinearity. The influence of pump laser parameters on EIG efficiency is also considered.

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Presenter: Doai Van Le

P.43 – Poster, VCTP-48

Dual-channel Optical bistability in a four-level atomic system with a static magnetic field

Le Van Doai, Luong Thi Yen Nga and Ho Hai Quang

Vinh University, 182 Le Duan Street, Vinh City, Vietnam.

Dual-channel Optical bistability in a four-level atomic system with a static magnetic field

Le Van Doai, Luong Thi Yen Nga and Ho Hai Quang Vinh University, 182 Le Duan Street, Vinh City, Vietnam. Email: doailv@vinhuni.edu.vn

Abstract: As we known that optical bistability (OB) is essential element in photonic devices such as optical transistors, optical memories, optical logic gates and optical switches, and so on [1]. Response speed and the sensitivity of the optical devices depend on the threshold intensity and width of the OB. Therefore, one is always looking for solutions to change the threshold intensity and the width of the OB, so that the operating characteristics of optical devices can be controlled. In recent years, the discovery of electromagnetically induced transparency (EIT) [2] has provided a simple solution to control both the threshold intensity and width of the OB can be easily controlled and reduced significantly [3]. Initially, theoretical and experimental studies on the OB focused on three-level atomic systems including three-level Ξ-, V- and ladder-type configurations [4-8]. It is found that, the threshold intensity and width of the OB system are controlled by the intensity and frequency of laser fields. Recently, Recently, many studies have been done to investigate optical bistability in four- and five-level atomic systems [9-11]. In this paper, we study the formation of a two-channel OB effect in a four-level atomic system in the presence of an external magnetic field. The OB effect is controlled according to the laser parameters and the external magnetic field.

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Presenter: Luong Thi Yen Nga

P.44 – Poster, VCTP-48

Double and triple occupancies in large mass imbalance mixtures

Thanh-Mai Thi Tran (1), Hong-Son Nguyen (2) and Minh-Tien Tran (1)

(1) Institute of Physics, Vietnam Academy of Science and Technology, Hanoi 10072, Vietnam;

(2) Department of Occupational Safety and Health, Trade Union University, 169 Tay Son, Hanoi, Vietnam

Optical lattices of dual-species atomic mixtures with large mass imbalance are modelled by an extended three-component Falicov-Kimball model. The dual-species mixtures consist of single-component light and double-component heavy atoms. Due to the large mass imbalance, only the light atoms are moveable across the optical lattice, whereas the heavy atoms are localized at the lattice sites. Both two- and three-body interactions between the atom components are included. The dynamics of light atoms, as well as the double and triple occupancies are determined within the dynamical mean field theory. It is found that the insulating phases can be classified by the double occupancies between the atom components, and they can occur only at certain fillings and strong interaction range. The triple occupancy is finite only in the metallic phase.

Presenter: Nguyễn Hồng Sơn

P.45 – Poster, VCTP-48

Electron-phonon correlations inducing excitonic excitations in semimetal and semiconducting materials

Do Thi Hong Hai (1) and Phan Van Nham (2)

(1) Department of Physics, Hanoi University of Mining and Geology, Duc Thang, Bac Tu Liem, Hanoi, Vietnam
(2) Institute of Research and Development, Duy Tan University, 3 Quang Trung, Danang, Vietnam

The influence of phonons on the low-energy excitonic excitations at zero temperature in the extended Falicov-Kimball model has been investigated. In the framework of the unrestricted Hartree-Fock approximation, a set of self-consistent equations for the excitonic condensate order parameter and a lattice distortion is derived when both electron-phonon coupling and electron-hole Coulomb interaction are treated on an equal footing. The low-energy excitation properties of the excitonic condensate are addressed in signatures of the optical conductivity and the dynamical excitonic susceptibility function. The real part of the optical conductivity is evaluated by the Kubo linear response theory and the imaginary part of the dynamical excitonic susceptibility is found by adapting the random phase approximation. In the semimetal state, one always finds a sharp peak in the optical conductivity spectrum indicating the stability of the excitonic condensation in the BCS type if the correlation between electrons and phonons becomes significant. In contrast, the peak is smeared out on the semiconducting side indicating the stability of the BEC-type excitonic condensate. In this semiconducting side, the sharp peak signature appears and the system turns to the BCS-type excitonic condensation state by increasing the electron-phonon correlations. In either the semimetal or the semiconducting normal state, increasing the electron-phonon correlations always reinforces a low-energy sharp peak in the dynamical excitonic susceptibility spectrum, indicating the existence of the tightly bound excitonic excitations before the condensation state. Specifically, on the semiconducting side, the "halo" phase with the preformed excitons exiting outside of the BEC-excitonic condensation state has been specified. The halo phase becomes more recognizable by raising the electron-phonon correlations.

Presenter: Do Thi Hong Hai

P.46 – Poster, VCTP-48

Excitonic insulator in the mass imbalance extended Falicov–Kimball model

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

(1) Department of Physics, Hanoi University of Mining and Geology, Duc Thang, Bac Tu Liem, Hanoi, Vietnam;
(2) Institute of Research and Development, Duy Tan University, 3 Quang Trung, Danang, Vietnam

Ground-state signatures of the excitonic insulator or excitonic condensation state in the mass imbalance extended Falicov-Kimball model in the presence of the electron-phonon correlation are investigated. Based on the unrestricted Hartree-Fock approximation, we have derived a set of self-consistent equations so the excitonic condensation order parameter is specified. The optical conductivity describing the low-energy excitations of the excitonic condensation state is considered in the Kubo linear response theory. At given sufficiently large electron-hole and electron-phonon couplings, phase diagrams show us the stability of the excitonic condensation state. The BCS-BEC crossover of the condensation state can be found in case of large mass imbalance. The BEC type of the condensate then disappears and one finds the simultaneous transition of the BCS condensate to the semimetal state by lowering the mass imbalance. Decreasing the electron-phonon coupling leads to the suppression of the excitonic condensate, specifically for the low mass imbalance. The influence of the electron-phonon interaction on the low-energy excitations of the excitonic condensate is also addressed in the signature of the real part of the optical conductivity.

Presenter: Nguyen Thi Hau

P.47 – Poster, VCTP-48

C4N3BN monolayer with persistent half-metallic magnetism

Pham Nam Phong (1), Huy-Viet Nguyen (2)

(1) School of Engineering Physics, Hanoi University of Science and Technology (HUST), 1 Dai Co Viet Road, Hanoi, Vietnam
(2) Institute of Physics, Vietnam Academy of Science and Technology (VAST), 10 Dao Tan Street, Hanoi, Vietnam

The new monolayer C_4N_3BN, short for triazine g-C_4N_3 with B and N tailored at vacant sites, is investigated under uniaxial or biaxial in-plane strain, with a focus on its ferrimagnetism. Our density functional study shows that the half-metallic nature of the material, together with its ferrimagnetic ground state, persists up to considerable strains from -7 to 10 percent, and temperatures as high as 900 K. Specifically, at the critical uniaxial strains of -9.30 and 10.90 percent, or symmetric biaxial strains of -7.62 and 17.38 percent, the monolayer undergoes four transitions to ferromagnetic order, all with a moment about 1 μ_B. We then present a simple explanation for this metamagnetism of the material by means of charge transfer and by counting its atomic valencies or bonding sequences in the unit cell. Our finding shows the importance and enriches the physicochemical understanding to the promising carbon nitride based half-metallic monolayers in spintronics.

Presenter: Phạm Nam Phong

P.48 – Poster, VCTP-48

Stationary characteristic quantities of contact interaction particle system in a harmonic trap or an optical lattice at extremely low temperature

Giau N. Nguyen (1), Khang M. Le (1), Uyen H.P. Mai (1), Thu D.H. Truong (1), Vinh N.T. Pham (1, 2)

(1) Department of Physics, Ho Chi Minh City University of Education, Ho Chi Minh City, Viet Nam.
(2) Office of Postgraduate Studies, Ho Chi Minh City University of Education, Ho Chi Minh City, Viet Nam.

In this study, the ground-state properties of a one-dimensional system of a small number of interacting bosons confined in a harmonic trap or optical lattice are numerically investigated. When the temperature is exceedingly low and the quantum gases are dilute, the two-body interacting potential is a delta-function-modeled contact interaction. In order to validate the numerical results, the Bose-Fermi mapping theorem is applied to derive the analytical solutions of this system at the extremity of its interaction and demonstrates satisfactory coincident.

Presenter: Pham Nguyen Thanh Vinh

P.49 – Poster, VCTP-48

Searching for AChE inhibitors from natural compounds by using machine learning and atomistic simulations

Quynh Mai Thai (a) , T. Ngoc Han Pham (a) , Dinh Minh Hiep (b), Minh Quan Pham (c,d) , Phuong-Thao Tran (e) , Trung Hai Nguyen (f,g) , Son Tung Ngo (a,h)

(a) Faculty of Pharmacy, Ton Duc Thang University, Ho Chi Minh City, Viet Nam
(b) Department of Agriculture and Rural Development, Ho Chi Minh City, Viet Nam
(c) Institute of Natural Products Chemistry, Vietnam Academy of Science and Technology, Hanoi, Viet Nam
(d) Graduate University of Science and Technology, Vietnam Academy of Science and Technology, Hanoi, Viet Nam
(e) Hanoi University of Pharmacy, 13-15 Le Thanh Tong, Hanoi, Viet Nam
(f) Laboratory of Theoretical and Computational Biophysics, Ton Duc Thang University, Ho Chi Minh City, Viet Nam
(g) Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Viet Nam
(h) Laboratory of Theoretical and Computational Biophysics, Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City, Viet Nam

Acetylcholinesterase (AChE) is one of the most important drug targets for Alzheimer's disease treatment. It hydrolyzes neurotransmitter acetylcholine resulting a deficiency of acetylcholine in brain and also common cause of Alzheimer's disease. Therefore, In this work, we used combined approach involving machine learning (ML) model and atomistic simulations (molecular docking, steeredmolecular dynamics simulations) was established to predict the ligand binding affinity of Vietnamese compounds to AChE. First, GraphConv model was selected and utilized to rapidly and accurately screen the natural compound database for potential AchE inhibitors. Then, atomic simulations were used to confirm that result, and 20 compounds be able to inhibit AChE were proposed through this good agreement. Especially, four compounds including geranylgeranyl diphosphate, 2-phosphoglyceric acid, and 2-carboxy-d-arabinitol 1-phosphate, and farnesyl diphosphate were predicted to be potential AChE inhibitors. These compounds with log(BB) in the range of -0.59 to 0.00 were able to cross the blood-brain barrier. Moreover, the hERG inhibition index showed that these compounds could not have toxicity to the human body. Overall, our obtained results may stimulate the search potentials drugs for an Alzheimer's disease therapy.

Presenter: Thai Quynh Mai

P.50 – Poster, VCTP-48

Re-investigation of heat capacity in some nuclei

Le Thi Quynh Huong (1), Nguyen Quang Hung (2,3), Nguyen Minh Hien (4), Tran Cong Duy(4)

(1) Department of Natural Science, University of Khanh Hoa, Nha Trang City, Khanh Hoa Province, Vietnam
(2) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 700000, Vietnam
(3) Faculty of Natural Sciences, Duy Tan University, Da Nang City 550000, Vietnam
(4) Graduate University of Sciences and Technology, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

The behavior of nuclear heat capacity in some nuclei is re-investigated by using the latest updated nuclear level density (NLD) data below the neutron binding energy B_n and the back-shifted Fermi-gas (BSFG) model with the energy-dependent level density parameter for the energy region above B_n. The new parameterization of the BSFG model has been proposed in order to obtain the best-fitted BSFG NLD in the entire region where the experimental data are available [1, 2, 3].

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Presenter: Le Thi Quynh Huong

P.51 – Poster, VCTP-48

Second order of perturbation theory as an analytical description for energy spectra of exciton in monolayer transition-metal dichalcogenides

Hanh T. Dinh, Ngoc-Hung Phan, Duy-Nhat Ly, and Van-Hoang Le

Ho Chi Minh City University of Education, Ho Chi Minh City, Vietnam

Two-dimensional exciton has currently been a subject of intensive studies by both theoretical and experimental approaches. In particular, the exciton energy spectra for s-state excitons in monolayer transition-metal dichalcogenides (TMDCs) were calculated numerically in most of the works (see, for example, [1-3]). However, their analytical expressions are also required for some physical analyses [4-5]. The Keldysh potential (for the screened electron-hole interaction) was obligatorily modified to obtain the analytical solutions in these works. Therefore, solutions achieved directly from the Schrodinger equation with the exact Keldysh interaction are still of great interest. We report some results of the regulatory perturbation theory (PT) method to solve the Schrodinger equation for excitons in monolayer TMDCs. Combining the FK operator method with the conventional perturbation theory allows a free parameter to regulate the convergence rate of the perturbation series. Consequently, the second approximation order of PT with an optimum choice of the free parameter gives accurate exciton energies for the 1s state with a relative error of less than 1% compared to the exact numerical solutions. This result inspires us

to use the solution obtained in the second order of PT as an analytical energy. We are continuing to apply this approach for higher excited states.

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Presenter: Dinh Thi Hanh

P.52 – Poster, VCTP-48

Investigating the Klein tunneling effect through a rectangular potential barrier in binary waveguide arrays

Minh C. Tran (1,2,3) and Truong X. Tran (4)

(1) Atomic Molecular and Optical Physics Research Group, Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Vietnam;
(2) Faculty of Applied Technology, School of Technology, Van Lang University, Ho Chi Minh City, Vietnam;
(3) Nuclear Training Center, VINATOM, 140 Nguyen Tuan street, Ha Noi, Vietnam;
(4) Department of Physics, Le Quy Don Technical University, 236 Hoang Quoc Viet street, Ha Noi, Vietnam.

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, which are higher than the energy of the particle, 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 investigated KT through a rectangular potential barrier in binary waveguide arrays. The rectangular potential step in this platform is created by introducing a certain offset for waveguides' refractive indices. We analytically derive the transmission coefficients of plane waves through the rectangular potential step in BWAs and also in the continuous model in free space [8]. 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

P.53 – Poster, VCTP-48

Study of the thermodynamic properties of SrTiO3 perovskite by the statistical moment method

Cao Huy Phuong

Hung Vuong University

We study the thermodynamic properties of cubic SrTiO3 perovskite going beyond the statistical moment method within approximation up to the fourth-order of the power moments of the atomic displacements. 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 SrTiO3, are obtained. The potential with the partial charge model and functions of Demontis and Pedone is used to calculate the numerical thermodynamic quantities of SrTiO3 from room temperature up to high temperature. The numerical results of the thermodynamic quantities of SrTiO3 by the statistical moment method are in good agreement with the previous theoretical and experimental results for a wide temperature range. Our research also shows that the anharmonic effects of the lattice fluctuations affect the thermodynamic properties of SrTiO3 dominantly. It has a good potential to develop the statistical moment method for investigating the temperature effects on the thermodynamic quantities of the perovskite–structure materials.

Presenter: Cao Huy Phuong

P.54 – Poster, VCTP-48

Dynamical entanglement and quantum teleportation via generalized photon-added pair coherent state under damping effect

Le Thi Hong Thanh (1,2), Truong Minh Duc (2)

(1) Quang Nam University, 102 Hung Vuong, Tam Ky City, Quang Nam Province, Viet Nam
(2) Center for Theoretical and Computational Physics, University of Education, Hue University, Hue City, Viet Nam

In this paper, we investigate the dynamical entanglement properties between an effective two-level atom and a field in generalized photon-added pair coherent state in the Jaynes-Cummings model under the influence of a damping effect. Besides, we introduce a field-atom entangled state applied for quantum teleportation of an unknown atomic state from a sender to a receiver which geographically distant. We use an average fidelity criterion to quantify this quantum teleportation process. In addition, we also compare the results in two cases with and without the damping effect. The results have shown that the dynamical entanglement and quantum teleportation process are influenced by the damping parameter.

Presenter: Le Thi Hong Thanh

P.55 – Poster, VCTP-48

The enhancement of Pauli blocking effect in odd-nuclei pairing

T. Vu Dong (1), L. Tan Phuc (2), N. Quang Hung(2), N. Dinh Dang (3), T. Dieu Huyen (4), N.L. Anh Tuan (4)

(1) University of Science, VNU-HCM
(2) Duy Tan University
(3) RIKEN Nishina Center for Accelerator-Based Science
(4) Ho Chi Minh City University of Education

Pairing reentrance in excited (hot) odd nuclei at low temperature (T<0.5-1 MeV) is caused by the weakening of Pauli blocking on the level occupied by the odd nucleon. At zero temperature, the single-particle occupation number of the last level occupied is 0.5 and it means this level is completely blocked. However, the proximity of neighboring levels to the odd level results in sharing the blocking property at a very low temperature, extending the blocking effect to the neighboring levels. Consequently, the levels surrounding the odd level can also be blocked, preventing pair-scattering processes. The diminishment or elimination of pairing reentrance occurs when Pauli blocking strongly influences the levels near the Fermi surface at low temperature.

Presenter: Tran Vu Dong

P.56 – Poster, VCTP-48

Hubbard parameters of Bi2O2Se from linear-response calculation

Do Quynh Anh (1) Nguyen Nhat Minh (2) Tran Van Quang (3)

(1) Hanoi-Amsterdam High School for the Gifted
(2) HUS High School for Gifted Students
(3) Faculty of Electronics and Telecommunications, VNU University of Engineering and Technology, Hanoi, Viet Nam

First-principles calculations based on density-functional theory (DFT) underestimate the bandgap of Bi2O2Se, known as a potential thermoelectric material. Advanced functionals, e.g, hybrid functional, GW, Koopmans-compliant functionals, etc, have been proposed to overcome this as a common issue. Recently, self-consistently determined onsite and intersite interactions by using linear-response calculation have been demonstrated to be effective in solving the bandgap problem. In this report, we present the results of calculations of the Hubbard U and V parameters, so-called DFT+U+V, by using linear response method and studying these effects on ground states of Bi2O2Se. We show that these effects can significantly improve the description of the excited states.

Presenter: Tran Van Quang

P.57 – Poster, VCTP-48

Impact of screening and relaxation in weakly coupled 2D macromolecular heterostructures: implications for switchable molecular spin-coupling

E. Rauls (1), T.T. Nhung Nguyen (2), T. Sollfrank (2), C. Tegenkamp (2), and U. Gerstmann (3)

(1) Institute of mathematics and physics, University of Stavanger;
(2) Institute of physics, TU Chemnitz;
(3) Theoretical physics, University of Paderborn

Phthalocyanines (Pc) at surfaces are prototype molecules which can host magnetic ions in a well-defined surface environment. The precise external control of the individual spins via electric fields, however, require a detailed knowledge of the influence of the substrate. In a combined experimental and theoretical study, we have investigated the structural and electronic properties

of Pb and Mn-phthalocyanines adsorbed on three different graphene-related substrates. Formation of almost identical densely packed PbPc molecular layers with strongly tilted molecules were found on both n-type and p-type doped 2D templates. On HOPG, in contrast, the dispersing molecular states of the less deformed molecular adsorbate stress the importance of substrate mediated interaction and proximity coupling [1]. Substituting Pb by Mn triggers the magnetic coupling within the molecular monolayer. The adsorption on either epitaxial or pyrolytic graphene leads to interesting differences in the adsorption behavior and the resulting electronic and magnetic properties. The different deformation ability of the vdW coupled systems, like their actual thickness and buckling, triggers the molecular morphology and exhibits a proximity coupled band structure. Like this, it provides important implications for future 2D design concepts of molecules at surfaces for sensing as well as information storage devices.

[1] T.T. Nhung Nguyen, T. Sollfrank, C. Tegenkamp, E. Rauls, U. Gerstmann, Phys. Rev. B 103, L201408 (2021).

Presenter: Rauls Eva

P.58 – Poster, VCTP-48

An upgrade to Lilith - a tool for constraining new physics from Higgs measurements

Nguyen Dang Bao Nhi (1), Le Duc Ninh (2), Sabine Kraml (3), Tran Quang Loc (4)

(1) University of Science, Vietnam National University, Ho Chi Minh City, Vietnam;
(2) Phenikaa University, Hanoi, Vietnam;
(3) Laboratoire de Physique Subatomique et de Cosmologie, Université Grenoble-Alpes, CNRS/IN2P3, Grenoble, France;
(4) She-Kings LLC, Santa Fe, US.

Lilith is a public Python library for constraining new physics from the Higgs production measurements by the statistical method of maximum likelihood. The current Lilith version 2.1 uses the Higgs signal strengths as input. This talk introduces a new version of the program, Lilith 2.2 coming with a new choice of input data using Simplified Template Cross Section (STXS) measurements. We then give examples of using Lilith to fit the Higgs couplings of the Standard Model Effective Field Theory and of the Two Higgs Doublet models type I and II for illustrating the usage of Lilith in various new physics scenarios. The importance of the theoretical uncertainties and their correlations on the constraint results is also discussed. The program is publicly available on GitHub.

Presenter: Nguyễn Đặng Bảo Nhi

P.59 – Poster, VCTP-48

Transmembrane Amyloid β-Peptide Structures: In Silico Study

Son Tung Ngo

Laboratory of Biophysics, Institute for Advanced Study in Technology, Ton Duc Thang University, Ho Chi Minh City, Vietnam

Amyloid beta (Aβ) peptides are considered the major causative agents of Alzheimer's disease (AD). In a widely accepted mechanism for AD pathogenesis, Aβ peptides are proposed to play multiple roles in damaging brain cells and their synaptic communications. Due to the heterogeneous nature Aβ oligomers, their in vivo structures have not been understood. Most experimental

and computational studies favored β-rich structures of Aβ as observed in Aβ fibrils. To determine the putative structures of the transmembrane Aβ oligomers, the temperature replica exchange molecular dynamics (REMD) simulations with an explicit solvent has been employed to monitor its structural change when the membrane DPPC lipid bilayers is induced. The initial structure of the oligomers was modelled based on the current low-resolution data of these conformations. The physical insights into the forming transmembrane Aβ oligomers probably enhance the AD therapy.

Presenter: Ngo Son Tung

P.60 – Poster, VCTP-48

Unlocking the Potential of GeS Monolayer: Strain-Enabled Control of Electronic Transports and Exciton Radiative Lifetimes

Vo Khuong Dien1, Pham Thi Bich Thao2, Nguyen Thi Han1, Nguyen Duy Khanh3, Le Vo Phuong Thuan1, Ming-Fa Lin1,4, and Nguyen Thanh Tien2

1 Department of Physics, National Cheng Kung University, 701 Tainan, Taiwan.

2 College of Natural Sciences, Can Tho University, 3-2 Road, Can Tho City 94000, Vietnam.

3 High-Performance Computing Laboratory (HPC Lab), Thu Dau Mot University, 75100, Binh Duong, Vietnam.

4 Hierarchical Green-Energy Material (Hi-GEM) Research Center, National Cheng Kung University, 701 Tainan, Taiwan.

Monolayer Germanium sulfide (GeS) is gaining significant attention for its exceptional anisotropic electronic conductance, notable excitonic effects, and wide range of potential applications. In our study, we used density functional theory (DFT), many-body perturbation theory (MBPT), and non-equilibrium Green's Function (NEGF) to investigate electronic transport properties and exciton radiative lifetime of single-layer GeS. Our theoretical findings showed that applying up to 8% compressive strain increased carrier mobility by nearly threefold, and thus, dramatically enhance the device's current intensity. Moreover, we observed that strain engineering allowed fine-tuning of the electron-hole recombination time. At 6% tensile strain, the effective radiative lifetime was as short as 19 picoseconds, which is 4.5 times faster than the intrinsic state and 80 times faster than at 8% compressive strain. These results highlight the potential of strain engineering to customize the electronic and optical properties of GeS monolayer for specific electronic, optoelectronic, and photovoltaic device requirements.

Presenter: Vo Khuong Dien

P.61 – Poster, VCTP-48

Observe muon decay with plastic scintillators, sipm, simplified electronics and data acquisition

Truong Thanh Sang (1), Cao Van Son (1), Pham Thuy Linh (1)

(1) The Institute For Interdisciplinary Research in Science and Education

We present a compact system for cosmic ray detection using Multi-Pixel Photon Counters (MPPC), an emerging type of Silicon Multiplier, a plastic scintillator, and simplified electronics for data acquisition. The coincidence technique was implemented to deal with the MPPC's intrinsic noise. The data acquisition is done directly from the oscilloscope via Ethernet offers us a flexibility in triggering and recording time window. The results of this study include mea-

surements of muon flow, muon light production, and observations of muon decay into electrons, presenting one experimental proof of the time dilation predicted by relativity theory. Our basic cosmic ray detection setup not only allows us to conduct particle experiments at a low cost, but it may also be used for muon radiography and tomography technology.

Presenter: Sang Thanh Truong

P.62 – Poster, VCTP-48

Effect of temperature on the compressibility in the semiconductor quantum well-wires

Le Van Tan

(1) Laboratory of Applied Physics, Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Vietnam;

(2) Faculty of Applied Technology, School of Engineering and Technology, Van Lang University, Ho Chi Minh City, Vietnam

In this article, we calculate the compressibility in GaAs semiconductor quantum well-wires that depends on both spin and finite temperature for different filling densities in the approximate PPA. We find that the compression ratio has the smallest value at filling density na = 1, and the compressibility increases as temperature and spin polarization increase

Presenter: Le Van Tan

P.63 – Poster, VCTP-48

The reconstruction of divacancies in zigzag-edge buckling silicene nanoribbons

Ngo Van Chinh (1,2), Pham Nguyen Huu Hanh (1,3), Nguyen Thi Kim Quyen (1,4), Vu Thanh Tra (5,6).

(1) School of Graduate, College of Natural Sciences, Can Tho University, 3/2 Street, Ninh Kieu District, Can Tho City, Vietnam;
(2) Ho Thi Ky High School, Ca Mau, Viet Nam;
(3) Thoi Thuan Middle and High School, Can Tho, Viet Nam;
(4) Faculty of Engineering and Technology, Kien Giang University, Kien Giang, Viet Nam;
(5) Department of Physics, School of Education, Can Tho University, Can Tho, Viet Nam;
(6) College of science, department of electrophysics, National Yangming Chiaotung University, Taiwan.

In this study, we utilized the tight-binding method to study the influence of a specific type of vacancy, specifically divacancies, on the electronic structure of zigzag-edge buckling silicene nanoribbons (ZBSiNRs). We employ the tight-binding approach to construct the atomic lattice of the ZBSiNRs with divacancies and subsequently calculate their electronic structure. Our study encompasses the following key aspects: (i) construction of the model and explanation of the corresponding material structure formation, (ii) examination of the influence of divacancy positions on material properties, (iii) investigate the influence of the external electric field on each type defect material properties. The results showed that, with a two-atom vacancy, depending on the vacancies and orientations, reconstructions can form types such as d5d7(double-5 double-7 structure), 585 (pentagon-octagon-pentagon structure), (t5t7- triple-5 triple-7 structure). Futhermore, The electronic properties of these materials are strongly dependent on the magnitude of electric field. These results are important to understand more comprehensively the

effects of external stimulus on the electronic properties of ZBSiNRs.

Presenter: Pham Nguyen Huu Hanh

P.64 – Poster, VCTP-48

Thermoelectric transport across a tunnel contact between two charge Kondo circuits

T. K. T. Nguyen(1), H. Q. Nguyen(1), and M. N. Kiselev(2)

(1) Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, 118000 Hanoi, Vietnam
(2) The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, I-34151, Trieste, Italy

Following a theoretical proposal on multi-impurity charge Kondo circuits [T.K.T Nguyen and M.N. Kiselev, Phys. Rev. B97, 085403 (2018)] and the experimental breakthrough in fabrication of the two-site Kondo simulator [W. Pouse et al, Nat. Phys (2023)] we investigate a thermoelectric transport through a two-site charge Kondo quantum nano-device in the strong coupling operational regime. We focus on the fingerprints of the non-Fermi liquid and its manifestation in the charge and heat quantum transport. We construct a full fledged quantitative theory describing crossovers between different regimes of the multi-channel charge Kondo quantum circuits and discuss possible experimental realizations of the theory.

Presenter: Nguyen Thi Kim Thanh

P.65 – Poster, VCTP-48

Studying and predicting Energy Gap of materials by Machine Learning Method

Le Huu Nghia (1) and Nguyen Thanh Tien (2)

(1) School of Graduate, Can Tho University, CanTho, Vietnam.
(2) College of Natural Sciences, Can Tho University.

Today, big data and artificial intelligence are revolutionizing many areas of our lives and the sciences. Materials science is not an exception, data-driven materials science is becoming the fourth paradigm of materials research, this report uses the Machine Learning method to find the best high-performance energy band gap in materials data. In this work, we start with data processing, analysis, modeling, and visualization of the results as well as a data organization process for machine learning models in materials research. We change the percentage of the dataset by setting a random seed from 0 to 60 (random. seed()) and find the best percentage for the data with train split = 70%; test split = 10%, and validation split = 20%. From the above percentage, our supervised machine learning finds the best-performing model: ExtraTreesRegressor() with the parameters: Coefficient of determination (R2): 0.7479, Mean Absolute Error (MAE): 0.5844, Root Mean Squared Error (RMSE): 0.8088. We consider therefore the different facets of interpretability prediction of models of machine learning and their importance in materials science. Finally, we propose solutions and future research paths for various challenges in computational materials science.

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Presenter: Le Huu Nghia

P.66 – Poster, VCTP-48

Thermodynamic properties of hcp structural metals under high pressure

Nguyen Thị Hong (1), Ho Khac Hieu (2), Tran Thi Hai (1), Nguyen Thi Dung (1)

(1) Hong Duc University, Thanh Hoa, Vietnam
(2) Duy Tan University, Da Nang, Vietnam

In this work, the Debye model has been developed to study the pressure dependence of the extended X-ray absorption fine structure Debye–Waller factor, the Debye frequency and temperature of hexagonal close-packed (hcp) metals. The effects of the non-ideal axial ratio c/a of hcp structure on these thermodynamic quantities at high temperatures and pressures have also been considered. Additionally, based on the combination of the Debye model and the Lindemann melting law, we derive the analytic expression of melting temperature of hcp metals as a function of pressure. Numerical calculations have been performed for Mg (up to 50 GPa) and Zn metals (up to 70 GPa). Our results are compared with those of previous experimental and theoretical data showing a good agreement. This verification of our developed theory allows us to believe that the current model can be widely applied to consider the pressure effects on the thermodynamic quantities of other materials.

Presenter: Nguyen Thi Hong

P.67 – Poster, VCTP-48

A DFT investigation of methanal gas absorption on monolayer MS_2 (M=W, Mo)

Quang Huy Tran (1), Thi Nhan Tran (2), Thi Theu Luong (3), Viet Bac Phung (4), Van An Dinh (5)

(1) 1Faculty of Physics, Hanoi Pedagogical University 2, Hanoi, Vietnam
(2) Faculty of Fundamental Sciences, Hanoi University of Industry, Hanoi, Vietnam
(3) Hoa Binh University, Hanoi, Vietnam
(4) VNU Vietnam Japan University, Luu Huu Phuoc, My Dinh I, Hanoi, Vietnam
(5) Department of Precision Engineering, Graduate School of Engineering, Osaka University, Osaka, Japan

Using density functional theory (DFT), this study explores the adsorption mechanism of methanal gas on the monolayer MS2 (M=W, Mo) surface. In order to characterize the adsorption of the gas molecule and its interaction with the MS_2 substrate, we utilize DFT simulations that incorporate van der Waals (vdW) interactions, conducted within the VASP framework. Using a Computational DFT-based Nanoscope tool, we determine the global minimum energy configurations and binding energies of gas molecules adsorbed on the monolayer MS_2. This allows us to visualize the various binding possibilities of gas molecules on the surface of MS_2. We compute the adsorption energy profiles using five functionals incorporating van der Waals interactions: revPBE-vdW, optPBE-vdW, vdW-DF2, optB88, and optB86b. The results reveal that the magnitude of adsorption energy decreases in the following order for both materials: optPBE $>$ optB88 $\approx$ optB86b $>$ revPBE $>$ vdW-DF2. Among the two materials, methanal exhibits higher sensitivity to the MoS_2 substrate, evidenced by its larger adsorption energy (253 meV) and a reduction in the bandgap (24 meV, equivalent to 1.1% decrease compared to non-adsorption). This study also includes in-depth discussions regarding the interaction between methanal and the MS_2 substrate, focusing on aspects such as charge transfer, modified density of states and band structure.

Presenter: Tran Quang Huy

List of Participants

Đỗ Mười
Pham Van Dong University
Email: dmuoi@pdu.edu.vn

Đỗ Quỳnh Anh
Hanoi-Amsterdam High School for Gifted
Email: dqa100606@gmail.com

Bach Huong Giang
VNU University of Science
Email: gbach@hus.edu.vn

Bach Thanh Cong
Faculty of Physics, VNU University of Science
Email: congbachthanh@gmail.com

Bui Dinh Hoi
Hue University of Education
Email: buidinhhoi@gmail.com

Cao Huy Phuong
Hung Vuong university
Email: caohuyphuongvlpt@yahoo.com.vn

Dang Minh Triet
Can Tho University
Email: dmtriet@ctu.edu.vn

Dang Van Soa
UNETI
Email: soadangvan@gmail.com

Dinh Thi Hanh
Ho Chi Minh City University of Education
Email: hanhdt@hcmue.edu.vn

Do Ngoc Son
Ho Chi Minh City University of Technology - VNU-HCM
Email: dnson@hcmut.edu.vn

Do Thi Hong Hai
Hanoi University of Mining and Geology
Email: dohonghaimdc@gmail.com

Doai Van Le
Vinh University
Email: doailv@vinhuni.edu.vn

Doan Quoc Khoa
The University of Danang - University of Science and Technology
Email: dqkhoa@dut.udn.vn

Duong Thi Man
Institute of Physics, VAST
Email: duongthiman28@gmail.com

Duy Tuấn Nguyễn
Institute of Physics
Email: ntduy@iop.vast.vn

Ho Hai Quang
hhquang96@gmail.com
Email: hhquangdhv@gmail.com

Ho Khac Hieu
Duy Tan University
Email: hieuhk@gmail.com

Ho Quoc Duy
Stavanger University
Email: duy.hoquoc@uis.no

Ho Sy Chuong
Dong Nai University
Email: hosichuong@gmail.com

Hoang Anh-Tuan
Institute of Physics - VAST
Email: hatuan@iop.vast.vn

Hoang Van Ngoc
Thu Dau Mot University
Email: ngochv@tdmu.edu.vn

Hoàng Trọng Đại Dương
Ho Chi Minh City University of Education
Email: hoangtrongdaiduong00@gmail.com

Huynh Anh Huy
Can Tho University
Email: hahuy@ctu.edu.vn

Huynh V. Phuc

Dong Thap Unversity
Email: hvphuc@dthu.edu.vn

Kim Hanchul
Sookmyung Women's University
Email: hanchul@sookmyung.ac.kr

Lapcharoensuk Ravipat
King Mongkut
Email: ravipat.la@kmitl.ac.th

Lê Mai Dũng
HNUE
Email: lmaidung@gmail.com

Lê Thị Hoá
Hue University of Education
Email: lethihoa.phys@gmail.com

Lý Duy Nhất
HCMC University of Education
Email: nhatld@hcmue.edu.vn

Le Duc Ninh
Phenikaa University
Email: ninh.leduc@phenikaa-uni.edu.vn

Le Van Hoang
Ho Chi Minh City University of Education
Email: hoanglv@hcmue.edu.vn

Le Dang Manh
Nguyen Tat Thanh University
Email: ledangmanh23696@gmail.com

Le Duc Vinh
Tinh Gia 3 high school
Email: leducvinhtg5@gmail.com

Le Huu Duc
Ho Chi Minh City University of Education
Email: lehuuduc2306@gmail.com

Le Huu Nghia
College of Natural Sciences - Can Tho University
Email: lehuunghiactu@gmail.com

Le Tan Phuc
Duy Tan University
Email: letanphuc191190@gmail.com

Le Thi Dieu Hien
University of Education, Hue University
Email: lehien32@husc.edu.vn

Le Thi Hong Thanh
Quang Nam University
Email: thanhle1008@gmail.com

Le Thi Quynh Huong
University of Khanh Hoa
Email: lethiquynhhuong@ukh.edu.vn

Le Van Tan
Van Lang University
Email: sobaobai@gmail.com

Luong Thi Yen Nga
Vinh University
Email: ngalty@vinhuni.edu.vn

Luu Tran Trung
University of Hong Kong
Email: ttluu@hku.hk

Lương Ngọc Thu Hà
HCMC University of Education
Email: thuhaluong2000@gmail.com

Lương Thị Thêu
Hoa Binh University
Email: 0989788471

Mineo Hirobumi
STAI, Van Lan University
Email: h_mineo@hotmail.com

Morikawa Yoshitada
Osaka University
Email: morikawa@prec.eng.osaka-u.ac.jp

Ngo Son Tung
Ton Duc Thang University
Email: sontungngo84@gmail.com

Ngo Van Chinh
Can Tho University
Email: ngovanchinhk13@gmail.com

Nguyễn Văn Chương

Học viện Kỹ thuật Quân sự
Email: chuong.vnguyen@lqdtu.edu.vn

Nguyễn Đặng Bảo Nhi
University of Science, VNU-HCM
Email: nguyendbaonhi@gmail.com

Nguyễn Hồng Sơn
Trường Đại học Công đoàn
Email: atvsld@gmail.com

Nguyễn Huy Việt
Institute of Physics, Vietnam Academy of Science and Technology
Email: nhviet@iop.vast.vn

Nguyễn Thị Hiền
The Institute For Interdisciplinary Research in Science and Education (IFIRSE)
Email: hiennt.bi11-077@st.usth.edu.vn

Nguyễn Thu Hương
Khoa khoa học cơ bản - Học viện phòng không không quân
Email: admin@hocvienpkkq.com

Nguyễn Trường Long
ĐH Cần Thơ
Email: truonglong@ctu.edu.vn

Nguyễn Văn Duy
Phenikaa Institute for Advaced Study and Faculty of Computer Science, Phenikaa University
Email: duy.nguyenvan@phenikaa-uni.edu.vn

Nguyễn Văn Hinh
Trường Đại học Công nghiệp Hà Nội
Email: nguyenvanhinh78@gmail.com

Nguyễn Duy Vỹ
Van Lang University
Email: nguyenduyvy@gmail.com

Nguyen Nhu Dat
Duy Tan University
Email: nguyennhudat@duytan.edu.vn

Nguyen Tri Lan
Institute of Physics
Email: ntlan@iop.vast.vn

Nguyen Ba Phi
Department of Basic Sciences, Mientrung University of Civil Engineering
Email: nguyenbaphi@muce.edu.vn

Nguyen Danh Tung
Viện vật lý
Email: ndtung@iop.vast.vn

Nguyen Dinh Nam
Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam
Email: nguyendinhnam@hus.edu.vn

Nguyen Hoang Linh
Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 700000, Vietnam
Email: hoanglinh221191@gmail.com

Nguyen Hong Quang
Institute of Physics, VAST
Email: nhquang@iop.vast.vn

Nguyen Huynh Kim Ngan
Institute of Fundamental and Applied Sciences, Duy Tan University
Email: ngannguyenqn79@hotmail.com

Nguyen Le Anh
Ho Chi Minh City University of Education
Email: anhnl@hcmue.edu.vn

Nguyen Mai Chung
University of Science and Technology of Hanoi (USTH)
Email: maichung.n@gmail.com

Nguyen Ngoc Hieu
Duy Tan University
Email: hieunn@duytan.edu.vn

Nguyen Quang Bau
Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam
Email: nguyenquangbau54@gmail.com

Nguyen Quang Hung

Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City
Email: nguyenquanghung5@duytan.edu.vn

Nguyen Quoc Thai
Dong Thap Unversity
Email: nqthai@dthu.edu.vn

Nguyen Quyet Thang
Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam
Email: qthang52@gmail.com

Nguyen Thanh Tien
Can Tho University
Email: nttien@ctu.edu.vn

Nguyen The Toan
University of Science, Vietnam National University
Email: toannt@hus.edu.vn

Nguyen Thi Hau
HaNoi University of mining and geology
Email: nguyenthihau@humg.edu.vn

Nguyen Thi Hong
Hong Duc university
Email: nguyenthihongvatly@hdu.edu.vn

Nguyen Thi Huong - Giang
Ho Chi Minh City University of Education
Email: nguyenthuonggiang00@gmail.com

Nguyen Thi Phuong Thuy
Institute of Physics, VAST
Email: ntpthuy@iop.vast.vn

Nguyen Thi Thao
Hanoi National University of Education
Email: thaont@hnue.edu.vn

Nguyen Thi Kim Thanh
Institute of Physics, VAST
Email: nkthanh@iop.vast.vn

Nguyen Thi Thu Trang
The University of Danang - University of Science and Technology
Email: ntthutrang@dut.udn.vn

Nguyen Tu Niem
VNU University of Science
Email: nguyentuniem@gmail.com

Nguyen Van Hoa
HCMUE
Email: hoanv@hcmue.edu.vn

Nguyen Vu Linh
Department of Theoretical Physics, Faculty of Physics and Engineering Physics, affiliated with the University of Science, Ho Chi Minh City
Email: 19130182@student.hcmus.edu.vn

Nguyen Xuan Thanh Tram
Division of Biomedical Engineering, Faculty of Applied Science, Ho Chi Minh City University of Technology, Ho Chi Minh City 70000, Vietnam Vietnam National University Ho Chi Minh City, Linh Trung Ward
Email: nxttram@hcmut.edu.vn

Nguyen-Truong Thanh Hieu
Dong Nai Technology University
Email: nguyentruongthanhhieu@dntu.edu.vn

Ong Phuong Khuong
Institute of High Performance Computing
Email: ongpk@ihpc.a-star.edu.sg

Pham Duy Kien
Ho Chi Minh City University of Education
Email: phamduykien32@gmail.com

Pham Nguyen Huu Hanh
Can Tho University
Email: hanhphamphysics@gmail.com

Pham Nguyen Thanh Vinh
Ho Chi Minh City University of Education
Email: vinhpnt@hcmue.edu.vn

Phan Nhut Huan
Institute of Fundamental and Applied Sciences, Duy Tan University
Email: phannhuthuan@duytan.edu.vn

Phan Thi Ngoc Loan
Ho Chi Minh City University of Education
Email: loanptn@hcmue.edu.vn

Phan To Quyen
IFIRSE
Email: phantoquyen97@gmail.com

Phan Van Nham
Duy Tan University
Email: phanvannham@duytan.edu.vn

Phạm Minh Trí
Phenikaa University
Email: 20010424@st.phenikaa-uni.edu.vn

Phạm Nam Phong
Hanoi University of Science and Technology
Email: phong.phamnam@hust.edu.vn

Phạm Thị Ngọc Hân
Viện kỹ thuật công nghệ cao Nguyễn Tất Thành
Email: ngochanpham274@gmail.com

Phạm Thị Thanh Nga
Trường Đại học Thủy lợi
Email: nga_ptt@tlu.edu.vn

Rauls Eva
University of Stavanger, Department of Mathematics and Physics
Email: eva.rauls@uis.no

Saurabh Prasoon
ECNU/Self
Email: psaurabh@uci.edu

Tang Thi Dien
VNU University of science
Email: tangthidien_sdh21@hus.edu.vn

Tống Sỹ Tiến
Trường Đại học Phòng cháy chữa cháy
Email: tongsytien@yahoo.com

Thai Quynh Mai
Ton Duc Thang University
Email: quynhmai150399@gmail.com

Tran Chien-Thang
Ho Chi Minh City University of Technology and Education
Email: thangtc@hcmute.edu.vn

Tran Nguyen Lan
International University, VNU-HCM
Email: tnlan@hcmiu.edu.vn

Tran Quang Dat
University of Transport and Communications-Campus in HCM City
Email: dattq_ph@utc.edu.vn

Tran Quang Huy
HPU2
Email: tranquanghuy@hpu2.edu.vn

Tran Thi Nhan
Hanoi University of Industry
Email: trannhan09@gmail.com

Tran Thi Thuy Linh
Institute of Fundamental and Applied Sciences, Duy Tan University
Email: trantthuylinh10@duytan.edu.vn

Tran Tuan Kha
Faculty of Computer Science and Pheninikaa Institute for Advanced Study, Phenikaa University
Email: kha.tt.carstairs@gmail.com

Tran Van Quang
Faculty of Electronics and Telecommunications, VNU University of Engineering and Technology
Email: tkuangv@gmail.com

Tran Viet Nhan Hao
Hue University
Email: tvnhao@hueuni.edu.vn

Tran Vu Dong
University of Science, VNU-HCM
Email: vudongti@gmail.com

Trần Anh Tuấn
Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam

National University, Hanoi, Vietnam.
Email: trananhtuan_sdh21@hus.edu.vn

Trần Công Minh
Science and Technology Advanced Institute, Van Lang University
Email: congminh96k40@gmail.com

Trần Minh Tiến
Institute of Physics
Email: minhtien@iop.vast.vn

Trieu Doan-An
Computational Physics Key Laboratory, Department of Physics, Ho Chi Minh University of Education
Email: kehy.antrieu@gmail.com

Trinh Xuan Hoang
Institute of Physics, VAST
Email: txhoang@iop.vast.vn

Truong Dang Hoai Thu
Ho Chi Minh city University of Education
Email: thutdh@hcmue.edu.vn

Truong Minh Duc
Hue University of Education
Email: tminhduc@hueuni.edu.vn

Truong Thanh Sang
The Institute For Interdisciplinary Research in Science and Education
Email: ttsang.phys@gmail.com

Vũ Hoàng Huy
Khoa Khoa học tự nhiên, Đại học Cần Thơ
Email: huym0821011@gstudent.ctu.edu.vn

Võ Hữu Cầu
Thanh Khe high school in Da nang city
Email: huucau.vl@gmail.com

Vo Khuong Dien
Researcher
Email: vokhuongdien@gmail.com

Vo Van Vien
Tay Nguyen University
Email: vvvien@ttn.edu.vn

Vu Ngoc-Tuoc
Hanoi University of Science and Technology
Email: tuoc.vungoc@hust.edu.vn

Vu Hoa Binh
Institude of Physics, VAST
Email: vhbinh@iop.vast.vn

Vu Thanh Tra
Can Tho University
Email: vttra@ctu.edu.vn

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Vietnam Academy of Science and Technology

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United Nations Educational, Scientific and Cultural Organization

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