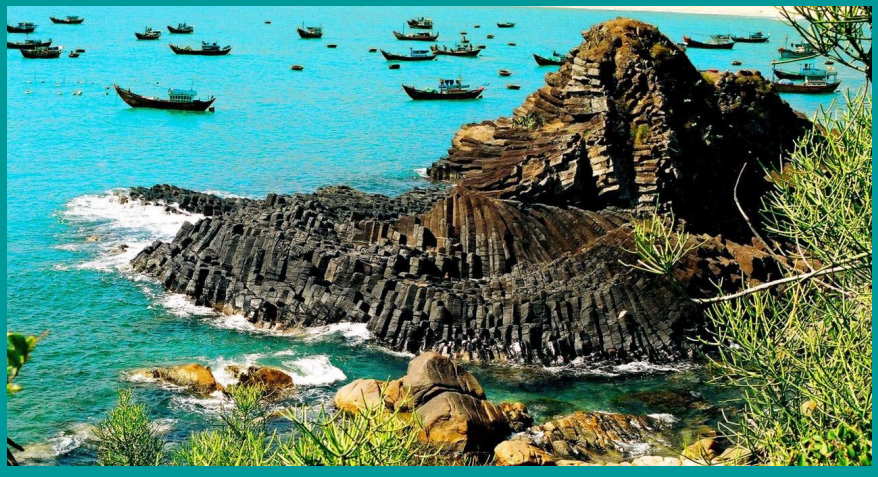
Program & Abstracts

47th Vietnam Conference on Theoretical Physics

HỘI NGHỊ VẬT LÝ LÝ THUYẾT VIỆT NAM LẦN THỨ 47



Tuy Hòa

1-4 August 2022

Program & Abstracts

47th Vietnam Conference on Theoretical Physics

Kaya Hotel
238 Hùng Vương,
Tuy Hòa, Việt Nam

1-4 August 2022

Contents

Welcome Message

It is a great pleasure to welcome you in the 47th Vietnam Conference on Theoretical Physics (VCTP-47).

The VCTP-47 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 South East Asia.

This year, the VCTP conference is participated by nearly 140 participants. 11 invited talks, 19 oral and 58 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

- Trinh Xuan Hoang (Institute of Physics, VAST), Chair
- Dinh Nguyen Dinh (Institute of Physics, VAST)
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Program Committee

- Tran Minh Tien (Institute of Physics, VAST), Chair
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- Nguyen The Toan (VNU University of Science, Hanoi)
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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-47 conference takes place in:

Kaya Hotel
238 Hùng Vương street
Tuy Hòa, Việt Nam

Instructions for offline/online participation

Offline participation

- Offline participation takes place at the conference site.

- Oral presenters present their talks as in a normal conference, except that the presentations will be broadcast via video conferencing for online participants.

- Poster presenters present the posters as in a normal conference, but they must also upload the PDF files of their posters to the conference website before the conference dates for online viewing.

Online participation

- Online participation takes place in Google Meet platforms.
- The link for each session will be posted on the program page of the conference website.
- All online presenters must join the online session before the session starts.
- The online sessions are coordinated by session chairs.
- Poster presenters must upload the PDF files of their posters to the conference website before the conference dates.
- Poster presenters will be asked by the poster session chair to show up online to answer questions of other participants.

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. A PDF file of the poster of size less than 5 MB must be uploaded to the conference website before the conference dates. Please follow the instructions on the conference website on how to present your poster online.

Meeting room

All sessions take place in the Harmonie conference room on the third floor of the Kaya Hotel. Please follow the direction in the lobby to go to the conference room.

Lunches

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

Gala dinner

All offline participants are invited to the Gala dinner:

Time: 3 August 2022, from 18:30 PM
Place: Kaya Hotel.

For your family members to attend the Gala Dinner, please buy tickets from the conference secretary on 1 August.

VTPS Meeting

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

Time: 17:30 PM - 18:00 PM, Monday, 1 August 2022.
Place: Harmonie Hall, 3rd floor, Kaya Hotel.

VTPS Young Research Award

At the opening session of the conference will be an announcement and the delivery of the 2022 VTPS Young Research Award.

Program timetable

Time	Monday, 1 August	Tuesday, 2 August	Wednesday, 3 August	Thursday, 4 August
08:30 – 10:00	Opening (8:30) VTPS Young Research Award Nguyen The Toan (I.1) Nguyen Hoang Linh (I.2) Photo Session *(Chair: Bach Thanh Cong)*	Poster Session 1 *(Chair: Hoang Anh Tuan)*	Excursion	Poster Session 2 *(Chair: Nguyen Thanh Tien)*
10:00 – 10:30	Coffee break	Coffee break		Coffee break
10:30 – 12:00	Cao Van Son (I.3) Tran Van Ngoc (O.1) Duong Van Loi (O.2) *(Chair: Hoang Ngoc Long)*	Le Anh-Thu (I.8) Trieu Doan An (O.5) Truong Dang Hoai Thu (O.6) *(Chair: Le Van Hoang)*		Senaha Eibun (I.10) Tran Viet Nhan Hao (O.12) Ngo Hai Tan (O.13) *(Chair: Nguyen Quang Hung)*
12:00 – 14:00	Lunch	Lunch		Lunch
14:00 – 15:30	Tran Nguyen Lan (I.4) Do Minh Hoat (O.3) Nguyen Thi Kim Thanh (O.4) *(Chair: Nguyen Toan Thang)*	Dao Thi Nhung (I.9) Le Truong My Hau (O.7) Le Van Dung (O.8) *(Chair: Phung Van Dong)*		Do Quoc Tuan (I.11) Nguyen Hoang Duy (O.14) Pham Manh Tuyen (O.15) *(Chair: Cao Hoang Nam)*
15:30 – 16:00	Coffee break	Coffee break		Coffee break
16:00 – 17:30	Nguyen Viet Hung (I.5) Nguyen Hai Son (I.6) Nguyen Duy Hoang Minh (I.7) *(Chair: Tran Minh Tien)*	Nguyen Lam Thuy Duong (O.9) Nguyen Duy Khanh (O.10) Nguyen Thi Kim Quyen (O.11) *(Chair: Nguyen Hong Quang)*		Nguyen Huynh Kim Ngan (O.16) Ho Quang Huy (O.17) Tran Cong Minh (O.18) Hoang Trong Dai Duong (O.19) *(Chair: Trinh Xuan Hoang)*
	VTPS Meeting (17:30)		Gala dinner (18:30)	Closing

Conference Program

Monday, 1 August 2022

Opening Session
Chair: Bach Thanh Cong, Trinh Xuan Hoang

08:30 - 08:35 Opening

08:35 - 08:40 Announcement of 2022 VTPS Young Research Award

08:40 - 09:20 I.1 – Invited
Asymptotic critical behavior of holographic superconductor phase transition — the spectrum of excited states becomes continuous at T = 0
Nguyen The Toan (University of Science, Vietnam National University, Hanoi)

09:20 - 10:00 I.2 – Invited
COVID-19: Molecular dynamics simulations
Nguyen Hoang Linh (Institute of Computational Science and Technology, Ho Chi Minh City)

10:00 - 10:05 Photo Session

10:05 - 10:30 Coffee break

Oral Session: *Particle, Nuclear and Astro- Physics*
Chair: Hoang Ngoc Long

10:30 - 11:10 I.3 – Invited
Latest results and prospects for the leptonic CP violation search in neutrino oscillation
Cao Van Son (Institute For Interdisciplinary Research in Science and Education)

11:10 - 11:35 O.1 – Oral
The possibility of discovering CPT violation with T2K-II, NOvA-II and JUNO
Tran Van Ngoc (IFIRSE)

11:35 - 12:00 O.2 – Oral
Novel effects of the W-boson mass shift in the 3-3-1 model
Duong Van Loi (Phenikaa University)

12:00 - 14:00 Lunch

Oral Session: *Condensed Matter Physics*
Chair: Nguyen Toan Thang

14:00 - 14:40 I.4 – Invited
New adventures in the development of electronic structure methods
Tran Nguyen Lan (National Institute of Applied Mechanics and Informatics)

14:40 - 15:05 O.3 – Oral
Exploration of new equiatomic quaternary Heusler compounds for spintronic applications
Do Minh Hoat (Institute of Theoretical and Applied Research, Duy Tan University)

15:05 - 15:30 O.4 – Oral
Cutler-Mott relation and Wiedemann-Franz law on a weak link between two charged Kondo circuits
Nguyen Thi Kim Thanh (Institute of Physics, VAST)

15:30 - 16:00 Coffee break

Oral Session: *Twistronics and Topology*
Chair: Tran Minh Tien

16:00 - 16:30 I.5 – Invited
Electronic properties and related features in twisted graphene systems
Nguyen Viet Hung (Université Catholique de Louvain)

16:30 - 17:00 I.6 – Invited
Strong coupling regime between a non-Hermitian topological charge and excitons in semiconductor
Nguyễn Hải Sơn (University of Lyon)

17:00 - 17:30 I.7 – Invited
Synthetic Weyl semimetal and quantum anomalous Hall state in a one-dimensional system of trilayer photonic grating
Nguyen Duy Hoang Minh (Donostia International Physics Center)

17:30 - 18:30 VTPS Meeting

Tuesday, 2 August 2022

Poster Session 1
Chair: Hoang Anh Tuan

08:30 - 10:00 P.1 – Poster
Field- and anisotropy-induced critical points and specific heat of XYZ ferromagnetic chain with single-ion anisotropy

Phạm Hương Thảo (Hue University of Education)

08:30 - 10:00 P.2 – Poster

Multiple returns in continuum harmonics of asymmetric molecules in multi-cycle lasers

Le Thi Cam Tu (Ton Duc Thang University)

08:30 - 10:00 P.3 – Poster

Retrieval of structural information of monolayer transition-metal dichalcogenides from exciton energy spectra

Ly Duy-Nhat (HCMC University of Education)

08:30 - 10:00 P.4 – Poster

Structural diversity and optoelectronic properties of chemical modification pentagonal quantum dots

Nguyen Thi My Hang (College Nature of seciences - Can Tho University)

08:30 - 10:00 P.5 – Poster

Effect of confined optical phonons on photo-stimulated Ettingshausen effect in rectangular quantum wires with a perpendicular field.

Cao Thị Vi Ba (VNU University of Science)

08:30 - 10:00 P.6 – Poster

Optimization of TiN-based ultraflexible materials for photothermal and solar harvesting applications

Do Thi Nga (Institute of Physics)

08:30 - 10:00 P.7 – Poster

Theoretical study of photostimulated Nernst effect in cylindrical quantum wires

Nguyen Thu Huong (Air Defense-Air Force Academy)

08:30 - 10:00 P.8 – Poster

Nested logistic map model: An application in immune system research

Nguyen Van Hoa (Ho Chi Minh City University of Education)

08:30 - 10:00 P.9 – Poster

The influence of partial boundary scattering on Seebeck coefficient oscillation in granular thermoelectric thin films

Bach Giang (VNU University of Science)

08:30 - 10:00 P.10 – Poster

Proton entropy excess and possible signature of pairing reentrance in hot nuclei

Nguyen Quang Hung (Institute of Fundamental and Applied Sciences, Duy Tan University)

08:30 - 10:00 P.11 – Poster

The new entanglement criterion for two-mode systems and application

Ho Sy Chuong (Dong Nai University)

08:30 - 10:00 P.12 – Poster
Mass-dependent binding energies of trions in parabolic quantum dots
Nguyen Que Huong (Marshall University)

08:30 - 10:00 P.13 – Poster
Zn-doped configurations in Germanene nanoribbons in electric field: A DFT study
Hoang Van Ngoc (Thu Dau Mot University)

08:30 - 10:00 P.14 – Poster
Magneto-optical responses in silicene.
Huynh V. Phuc (Dong Thap University)

08:30 - 10:00 P.15 – Poster
A first-principles investigation of methanal gas absorption on WS2 monolayer
Huy Tran Quang (Hanoi Pedagogical University 2)

08:30 - 10:00 P.16 – Poster
Exciton behaviors in monolayer WSe_2 under isotropic strain
Tran Thị Nhan (Hanoi University of Industry)

08:30 - 10:00 P.17 – Poster
One-loop contribution for $H \to ZZ^* \to Z\ f\ f$ in Standard Models
Trần Trí Dũng (Ho Chi Minh City University of Science)

08:30 - 10:00 P.18 – Poster
The characteristic frequency equation and the semi-empirical formula for the coupling strength in cantilever array
Le Tri Dat (Ton Duc Thang University)

08:30 - 10:00 P.19 – Poster
Role of thermal quantities in framework of nuclear pairing correlation
Le Tan Phuc (Institute of Fundamental and Applied Sciences, Duy Tan University)

08:30 - 10:00 P.20 – Poster
Grafting Methionine on 1F1 Antibody Increases the Broad-Activity on HA Structural-Conserved Residues of H1, H2, and H3 Influenza A Viruses
Lê Thanh Hòa (Advanced Institute of Materials Science, Tôn Đức Thắng University)

08:30 - 10:00 P.21 – Poster
Electron transport through experimentally controllable parabolic bubbles on graphene nanoribbons
Nguyen Mai Chung (University of Science and Technology of Hanoi)

08:30 - 10:00 P.22 – Poster
Toward multi-target drug therapeutic of Chronic obstructive pulmonary disease: In silico study of Ergosterol using molecular docking, molecular dynamics simulation and binding free energy

Do Tuan (Phenikaa University)

08:30 - 10:00 P.23 – Poster
Islands in regular black strings
Tran Ngoc Hung (Phenikaa University)

08:30 - 10:00 P.24 – Poster
Edge states in a model of magnetic topological insulators
Nguyễn Hồng Sơn (Trường Đại học Công đoàn)

08:30 - 10:00 P.25 – Poster
Divacancy effects on the electronic properties of zigzag buckling silicene nanoribbons
Pham Nguyen Huu Hanh (Can Tho University)

08:30 - 10:00 P.26 – Poster
Feature-rich structural and electronic properties of halogen-functionalized germanene nanoribbons: A DFT study
Vo Van On (Thu Dau Mot University)

08:30 - 10:00 P.27 – Poster
Optical refraction and absorption spectra in perturbed monolayer PbBiI
Le Thi Thu Phuong (Hue University of Education)

08:30 - 10:00 P.28 – Poster
Effect of gate voltage on the anisotropic optical transitions of β_{12}-borophene
Bui Dinh Hoi (Hue University of Education)

08:30 - 10:00 P.29 – Poster
Energy of hydrogen atom in excited states induced by static electric field
Pham Quang Huy (Ho Chi Minh City, University of Education)

08:30 - 10:00 P.30 – Poster
The interaction between Bose – Einstein Condensate fluid and fixed potential wall
Pham Nguyen Thanh Vinh (Ho Chi Minh City University of Education)

10:00 - 10:30 Coffee break

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

10:30 - 11:10 I.8 – Invited
Novel strong-field techniques for probing ultrafast processes in atoms and molecules
Anh-Thu Le (University of Connecticut)

11:10 - 11:35 O.5 – Oral
Extracting terahertz time domain using high-order harmonic generation
Trieu Doan An (Computational Physics Laboratory, Department of Physics, Ho Chi Minh University of Education)

11:35 - 12:00 O.6 – Oral

The soft parameter of attractive Coulomb potential in nonsequential double ionization process

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

12:00 - 14:00 Lunch

Oral Session: *Particle, Nuclear and Astro- Physics*
Chair: Phung Van Dong

14:00 - 14:40 I.9 – Invited

The Inverse Seesaw mechanism and its impacts on the Higgs sector and lepton's anomalous magnetic moments

Dao Thi Nhung (Phenikaa University)

14:40 - 15:05 O.7 – Oral

The neutrino masses and theirs effects on the Higgs sector of the Next-toTwo Higgs Doublet Model including Inverse Seesaw mechanism

Le Truong My Hau (Ho Chi Minh City University of Science)

15:05 - 15:30 O.8 – Oral

Unparticle effects at the MUonE experiment

Le Van Dung (Ho Chi Minh City University of Science)

15:30 - 16:00 Coffee break

Oral Session: *Condensed Matter Physics*
Chair: Nguyen Hong Quang

16:00 - 16:25 O.9 – Oral

Correlation between energy band transition and optical absorption spectrum in bilayer armchair graphene nanoribbons

Nguyen Lam Thuy Duong (Can Tho University)

16:25 - 16:50 O.10 – Oral

Halogenation effects in silicene and silicene nanoribbons: A DFT study

Nguyen Duy Khanh (High-Performance Computing Laboratory (HPC Lab), Thu Dau Mot University)

16:50 - 17:15 O.11 – Oral

Bilayer armchair graphene nanoribbons under the effect of combining vacancy and external electric fields

Nguyen Thi Kim Quyen (CanTho University)

Wednesday, 3 August 2022

08:00 - 16:00 Excursion

18:30 - 20:30 Gala dinner

Thursday, 4 August 2022

Poster Session 2
Chair: Nguyen Thanh Tien

08:30 - 10:00 P.31 – Poster

Applying first principle to study the structure, electrical and optical properties of Sc adsorbed ASiNRs

Nguyen Thanh Tung (Thu Dau Mot University)

08:30 - 10:00 P.32 – Poster

One-loop contributions to the decay processes $H \to f f^{-}\gamma$ in beyond the Standard Model.

Phan Hong Khiem (Institute of Fundamental and Applied Sciences, Duy Tan University)

08:30 - 10:00 P.33 – Poster

Ferromagnetic Magnon in Monolayer Honeycomb Spin Lattice in The Application of Transverse Field

Nguyễn Từ Niệm (VNU University of Science)

08:30 - 10:00 P.34 – Poster

Entanglement, nonlocality, quantum teleportation of two-mode non-Gaussian states with multiphoton quantum catalysis

Tran Quang Dat (University of Transport and Communications)

08:30 - 10:00 P.35 – Poster

Study of the thermodynamic properties of BaTiO3 perovskite by the statistical moment method with improved interatomic potential.

Cao Huy Phuong (Hung Vuong University)

08:30 - 10:00 P.36 – Poster

Open Kondo circuit as a detector for electron-electron interactions in a Luttinger Liquid

Nguyễn Hồng Quang (Viện Vật lý, Viện Hàn lâm KH&CN Việt Nam)

08:30 - 10:00 P.37 – Poster

Stability, geometrical and electronic structures of the mixed aluminum – scandium clusters AlxScy, with x + y = 13

Nguyen Minh Tam (Ton Duc Thang University)

08:30 - 10:00 P.38 – Poster

Phase diagram of the half-filled disordered Hubbard model at finite temperature

Hoang Anh Tuan (Institute of Physics, VAST)

08:30 - 10:00 P.39 – Poster

First-principles insights into the Janus group III monochalcogenides

Nguyen Ngoc Hieu (Duy Tan University)

08:30 - 10:00 P.40 – Poster

Structural, electronic properties of pentagonal $PdSe_2$ nanoribbons: a first-principles calculations

Nguyen Thanh Tien (College of Natural Sciences, Can Tho University)

08:30 - 10:00 P.41 – Poster

Conductivity in the disordered Hubbard model at half-filling

Nguyen Thi Hai Yen (Institute of Physics, VAST)

08:30 - 10:00 P.42 – Poster

Neutrino mass spectrum with the present neutrino data

Phan To Quyen (Institute For Interdisciplinary Research in Science and Education)

08:30 - 10:00 P.43 – Poster

Magnon spectrum of the spin-1 J1 –J2 antiferromagnetic Heisenbeberg model on a triangular lattice

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

08:30 - 10:00 P.44 – Poster

A molecular dynamics simulations of penta silicene anoribbons affected by size, edge and pressure

Trang Như Hải (Can Tho University)

08:30 - 10:00 P.45 – Poster

Size, type boundary and pressure effect on silicene nanoribbons by molecular dynamics simulation

Nguyễn Thị Bích Doanh (Can Tho University)

08:30 - 10:00 P.46 – Poster

Entanglement and quantum teleportation with nonlinear charge pair cat states

Dang Huu Dinh (Industrial University of Ho Chi Minh City)

08:30 - 10:00 P.47 – Poster

Investigation of pairing phase transition in some excited meadium nuclei

Le Thi Quynh Huong (University of Khanh Hoa)

08:30 - 10:00 P.48 – Poster

Extracting asymmetricity of polar molecular from high order harmonic generation: effect of partial orientation

Phan Ngoc-Loan (Ho Chi Minh City University of Education)

08:30 - 10:00 P.49 – Poster

Functional integral approach for the Heisenberg model: beyond one-loop approximation

Pham Thi Thanh Nga (Thuyloi University)

08:30 - 10:00 P.50 – Poster

Quantum teleportation of entangled states via generalized photon-added pair coherent state

Le Thi Hong Thanh (Quang Nam University)

08:30 - 10:00 P.51 – Poster

A first-principles investigation of toxic gases absorption on MoSe2 monolayer

Luong Thi Theu (Institute of Sustainability Science, VNU Vietnam Japan University)

08:30 - 10:00 P.52 – Poster

Effects of hydrophobic and electrostatic interactions on the escape of proteins at archaeal and bacterial ribosomal exit tunnels

Bui Phuong Thuy (Institute of Theoretical and Applied Research, Duy Tan University)

08:30 - 10:00 P.53 – Poster

Can DNA form twisted bundles in toroidal condensates?

Nguyễn Thị Thùy Nhung (Institute of Physics, VAST)

08:30 - 10:00 P.54 – Poster

Indentifying the key sites for the thermal stability of glucose-6-phosphate dehydrogenase from a structure-based model

Trinh Xuan Hoang (Institute of Physics, VAST)

08:30 - 10:00 P.55 – Poster

Physics implication from a Z_3 symmetry of hadrons

Phung Van Dong (Phenikaa University)

08:30 - 10:00 P.56 – Poster

Investigating the structural features of SRAS-CoV-2 Mpro binding site bound covalent ligands at physiological temperature

Nguyễn Thế Toàn (University of Science, Vietnam National University, Hanoi)

08:30 - 10:00 P.57 – Poster

Studying the effect of structure on the dynamics in MgSiO4 by a molecular dynamics simulation

Giap Thi Thuy Trang (Thai Nguyen University of Education)

08:30 - 10:00 P.58 – Poster

H2 physisorption on the internal surface of metal organic framework MOF-74 based materials by ab initio molecular dynamics simulation

Nguyen Thuy Trang (University of Science, Vietnam National University)

10:00 - 10:30 Coffee break

Oral Session: *Particle, Nuclear and Astro- Physics*
Chair: Nguyen Quang Hung

10:30 - 11:10 I.10 – Invited

A renormalization group improvement for thermally resummed effective potential

Senaha Eibun (Van Lang University)

11:05 - 11:30 O.12 – Oral

Coulomb divergence in (d,p) reactions based on the Faddeev-Alt-Grassberger-Sandhas equation

Trần Viết Nhân Hào (Faculty of Physics, University of Education, Hue University)

11:35 - 12:00 O.13 – Oral

Spin symmetry energy and equation of state of spin-polarized neutron star matter

Ngo Hai Tan (Phenikaa University)

12:00 - 14:00 Lunch

Oral Session: *Particle, Nuclear and Astro- Physics*
Chair: Cao Hoang Nam

14:00 - 14:40 I.11 – Invited

No-go theorem for inflation in Ricci-inverse gravity

Do Quoc Tuan (Phenikaa University)

14:40 - 15:05 O.14 – Oral

On the anisotropic constant-roll inflation for the Dirac-Born-Infeld model

Nguyen Hoang Duy (Phenikaa Institute for Advanced Study, Phenikaa University and Graduate University of Science and Technology, Vietnam Academy of Science and Technology)

15:05 - 15:30 O.15 – Oral

A novel k-Gauss-Bonnet power-law inflation model

Pham Manh Tuyen (Phenikaa Institute for Advanced Study, Phenikaa University, and Graduate University of Science and Technology, Vietnam Academy of Science and Technology)

15:30 - 16:00 Coffee break

Oral Session: *Molecular Physics, Quantum Optics, and Quantum Information*
Chair: Trinh Xuan Hoang

16:00 - 16:25 O.16 – Oral

A method for retrieving asymmetricity of polar molecule from high harmonic generation

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

16:25 - 16:50 O.17 – Oral

Generation of dynamic stark-induced degenerate vibronic state by two shift up non-resonant lasers

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

16:50 - 17:15 O.18 – Oral

Investigating the inverse Klein tunneling effect in binary waveguide arrays

	Trần Công Minh (Van Lang University)
17:15 - 17:40	O.19 – Oral Construction molecular potential using machine learning **Hoàng Trọng Đại Dương** (Ho Chi Minh City University of Education)
17:40 - 17:50	Closing

Conference Abstracts

I.1 – Invited, VCTP-47

Asymptotic critical behavior of holographic superconductor phase transition — the spectrum of excited states becomes continuous at T = 0

Toan T. Nguyen (1) and Tran Huu Phat (2)

(1) Key Laboratory for Multiscale Simulation of Complex Systems and Department of Theoretical Physics, University of Science, Vietnam National University – Hanoi, 334 Nguyen Trai street, Thanh Xuan, Hanoi, 100000, Vietnam (2) Vietnam Atomic Energy Commission, 59 Ly Thuong Kiet street, Hoan Kiem, Hanoi, 100000, Vietnam

Within the framework of AdS/CFT duality, excited states of the conformal field living at the global AdS boundary of a four-dimensional spacetime Einstein gravity are investigated analytically in the probe limit where the field equations are linearized. At asymptotically large values, the threshold chemical potential for the appearance of excited condensate states are discrete, equal spacing, with the gap approaches zero logarithmically in the limit $T \to 0$. Remarkably, numerical results show that, this behavior applies even for states as low as for the first or the second excited state of the condensate. This is especially significant on the liquid side of the black hole van der Waals-like phase transition (small or zero topological charge) where there seems to be no gap between the ground state and the first excited state at zero temperature. We postulate that, at the exact limit $T = 0$ where the gap is zero, the spectrum of threshold chemical potentials becomes continuous, all excited states of the condensate are activated above a finite chemical potential, suggesting a new quantum phase transition as a function of the chemical potential. Previous studies have largely missed this continuous spectrum of excited states in the $T \to 0$ limit. This fact should be taken into account carefully in AdS/CFT duality studies.

Presenter: Nguyen The Toan

I.2 – Invited, VCTP-47

COVID-19: Molecular dynamics simulations

Hoang Linh Nguyen (1,2,3), Nguyen Quoc Thai (1,4), Phuong H. Nguyen (5) and Mai Suan Li (6)

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The 2019 novel coronavirus (SARS-CoV-2) epidemic, which was first reported in December 2019 in Wuhan, China, was declared a pandemic by the World Health Organization in March 2020. Genetically, SARS-CoV-2 is closely related to SARS-CoV, which caused a global epidemic with 8096 confirmed cases in more than 25 countries from 2002 to 2003. Given the significant morbidity and mortality rate, the current pandemic poses a danger to all of humanity, prompting us to understand the activity of SARS-CoV-2 at the atomic level. Experimental studies have revealed that spike proteins of both SARS-CoV-2 and SARS-CoV bind to angiotensin-converting enzyme 2 (ACE2) before entering the cell for replication. However, the binding affinities reported by different groups seem to contradict each other. To understand the binding mechanism and experimental results, we investigated how the receptor binding domain (RBD) of SARS-CoV (SARS-CoV-RBD) and SARS-CoV-2 (SARS-CoV-2-RBD) interacts with a human ACE2-PD using molecular modeling. Using steered all-atom molecular dynamics simulations, we demonstrate that, like a coarse-grained simulation, SARS-CoV-2-RBD was associated with ACE2-PD more strongly than was SARS-CoV-RBD, as evidenced by a higher rupture force and larger pulling work. We show that the binding affinity of both viruses to ACE2 is driven by electrostatic interactions.

Presenter: Nguyen Hoang Linh

I.3 – Invited, VCTP-47

Latest results and prospects for the leptonic CP violation search in neutrino oscillation

Son Cao

Institute For Interdisciplinary Research in Science and Education

All three of the known unknowns in particle physics are related to neutrinos. One of them is the leptonic CP violation, and physicists are excited by the recent T2K experiment indication on this mirror breaking. The talk will provide an update on the latest results from two flagship experiments, the T2K experiment in Japan and the NOvA experiment in the United States. We also talk about the prospects of uncovering this unknown over the next decade.

Presenter: Cao Van Son

I.4 – Invited, VCTP-47

New adventures in the development of electronic structure methods

Tran Nguyen Lan

Institute of Applied Mechanics and Informatics, VAST

The theoretical description of the electronic structure of complex molecules and materials faces two main challenges. First, the size of simulated systems needs to be large enough to remove the artificial effects caused by the finite size. Second, many-body effects need to be described accurately. While high-level methods can tackle the latter, their high computational costs limit them to small-size simulated systems. On the other hand, while low-cost methods like density functional theory can deal with large-size systems, they are usually unable to provide a satisfactory accuracy for systems with strong many-body effects. Therefore, methods that can balance cost and accuracy are highly desirable. In this talk, I will present some electronic-structure

methods that we are currently developing in our lab: self-consistent perturbation theory, hybrid quantum-classical framework, and neural-network quantum states.

Presenter: Tran Nguyen Lan

I.5 – Invited, VCTP-47

Electronic properties and related features in twisted graphene systems

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In recent years, stacking two-dimensional crystals to form new materials has proved relatively easy, as the van der Waals forces between successive layers are weak, to explore a broad range of novel physical and chemical properties [1]. Furthermore, this versatile method adds some degrees of freedom which can be exploited to devise heterostructures with new properties, different from the simple combination of properties of the individual materials forming the stack. Remarkably, the misorientation (characterized by the twist angle) and/or lattice mismatch between successive 2D crystals creates long-range super-periodicity known as moiré [2,3]. The effect of the twist angle and its associated moiré is particularly spectacular when considering electrical, magnetic and optical properties. In particular, twisted bilayer graphene can switch from insulating to superconducting, or to more exotic quantum or topological phases due to strong electronic correlations at low twist angle. Such observations have been considered as real scientific breakthroughs, creating a nascent field of "twistronics" [4], i.e. aiming to explore novel physical properties in vertically stacked 2D structures when tuning the twist angle between the related layers. In this talk, we will present an overview of our recent researches [5-8] related to the electronic properties of twisted graphene systems. These researches centred on the understanding of the interplay between atomic-scale structure (i.e., created moiré superlattices) and electronic properties in the mentioned twisted systems.

References: [1] A. Geim and I. Grigorieva, Van der Waals heterostructures, Nature 499, 419-425 (2013). [2] E. Y. Andrei and A. H. MacDonald, Graphene bilayers with a twist, Nat. Mater. 19, 1265-1275 (2020). [3] F. He, Y. Zhou, Z. Ye, S.-H. Cho, J. Jeong, X. Meng, and Y. Wang, Moiré Patterns in 2D Materials: A Review, ACS Nano 15, 5944-5958 (2021). [4] Z. Hennighausen and S. Kar, Twistronics: a turning point in 2D quantum materials, Electron. Struct. 3, 014004 (2021). [5] A.C. Gadelha, D. A. A. Ohlberg, C. Rabelo, et al., Localization of lattice dynamics in low-angle twisted bilayer graphene, Nature 590, 405-409 (2021). [6] V. Hung Nguyen, et al., Electronic localization in small-angle twisted bilayer graphene, 2D Mater. 8, 035046 (2021). [7] A. C. Gadelha, V. Hung Nguyen, et al., Electron-phonon coupling in a magic-angle twisted-bilayer graphene device, arXiv:2110.14916 (2021). [8] V Hung Nguyen, et al., Electronic properties of twisted multilayer graphene, J. Phys. Mater. 5, 034003 (2022).

Presenter: Nguyen Viet Hung

I.6 – Invited, VCTP-47

Strong coupling regime between a non-Hermitian topological charge and excitons in semiconductor

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Non-perturbative radiation-matter coupling between dipole-active material excitations and confined modes of the electromagnetic field leads to the concept of polaritons, i.e., hybrid excitations of mixed nature involving at least two fields with different characteristics [1]. Exciton-polaritons, in particular, are mixed light-matter excitations resulting from the strong coupling regime between exciton in semiconductors and confined photons. Harnessing these hybrid excitations provides a rich playground to explore fascinating fundamental features, as out-of-equilibrium Bose-Einstein condensation and quantum fluids of light, plus novel mechanisms to be exploited in optoelectronic devices. In this talk, I will present the theory and experimental realizations of the strong coupling regime between excitons in quantum wells and a peculiar confined photon state called Bound state In a Continuum (BIC). BICs are peculiar localized states that are forbidden to radiate despite lying in a continuum of propagating waves [2]. These states were first predicted by Von Neumann and Wigner in 1929, and were once regarded as an "exotic" quantum mechanical effect. The origin of BICs is nowadays fully unraveled as a particular solution of wave equations, which has led to their exploitation in other fields where it is straightforwardly attributed to destructive interference mechanisms or symmetry mismatches. Interestingly, each photonic BIC in an optical lattice is attributed to a topological charge pinned at a polarization singularity in the momentum space [2]. This topological nature will be perfectly transferred to the polaritonic states once the strong coupling regime is established. As proofs of concept, I will show the experimental demonstration of a Bose Einstein condensation in a polariton bound state in the continuum [3]. This macroscopic states has been achieved with traditional inorganic quantum wells at cryogenic temperature. Finally, I will present the first demonstration demonstration of polariton BIC at room temperature using hybrid organic-inorganic quantum wells [4].

References :

[1] D. N. Basov et al., "Polariton panorama", Nanophotonics, 10, 549-577, 2021.

[2] C. W. Hsu et al., "Bound states in the continuum," Nature Reviews Materials, 1, 16048, 2016

[3] V. Ardizzone et al., "Polariton Bose-Einstein condensate from a bound state in the continuum," Nature, 605, 447-452, 2022.

[4] N. H. M. Dang et al., "Realization of polaritonic topological charge at room temperature using polariton bound states in the continuum from perovskite metasurface," Advanced Optical Materials, 10, 2102386, 2022.

Presenter: Nguyễn Hải Sơn

I.7 – Invited, VCTP-47

Synthetic Weyl semimetal and quantum anomalous Hall state in a one-dimensional system of trilayer photonic grating

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We study the spectral properties of a one-dimensional (1D) trilayer photonic grating in a 3D

hybrid momentum space, where the interlayer shifts play the role of two synthetic momenta besides the conventional momentum of our 1D system. As the synthetic momenta are even under the time-reversal operation, this family of 1D lattice can host states that are realized in systems with broken time-reversal symmetry. We find that highly tunable Weyl semimetal, nodal line semimetal, and quantum anomalous Hall state can be realized in such a trilayer waveguide. The results show that multilayer photonic grating is not only a promising platform for studying higher-dimensional topological physics but also a simple one for observeing interface states between 3D systems, which is difficult in condensed matter physics.

Presenter: Nguyen Duy Hoang Minh

I.8 – Invited, VCTP-47

Novel strong-field techniques for probing ultrafast processes in atoms and molecules

Anh-Thu Le

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In ultrafast chemical reactions, electrons and nuclei in molecules move at attosecond and femtosecond timescales on multidimensional landscapes called potential energy surfaces (PES). Understanding and controlling their complex coupled motions and the outcome of chemical reactions has been a dream of quantum physicists. Recent progress in laser technology has led to new coherent light sources that can be used to investigate ultrafast processes in matter. To take advantage of these new light sources, different experimental techniques have been developed to reveal the inner-workings of coupled electron-nuclear dynamics in molecules. Concurrently, theoretical and computational tools have also been developed to understand and decode hidden information from the experimental measurements. In this talk, I will first review some of those advancements. I will then present our group's recent progress in understanding intense laser-atom/molecule interactions by using some of the most promising techniques such as laser-induced electron diffraction, high-harmonic generation spectroscopy, and attosecond transient absorption spectroscopy. Throughout the talk, I will also address the challenges and opportunities in this field for practical realization of molecular "movies" with atomic resolution in space and time that can provide new insights into fundamental chemical reactions.

Presenter: Anh-Thu Le

I.9 – Invited, VCTP-47

The Inverse Seesaw mechanism and its impacts on the Higgs sector and lepton's anomalous magnetic moments

Dao Thi Nhung

Phenikaa University

The extended (s)neutrino sector can explain the small active neutrinos masses via the inverse seesaw mechanism, while still allows for large values of the neutrino Yukawa couplings with a mass scale of sterile neutrinos of order TeV. They can affect the Higgs sector, lepton's anomalous magnetic moments and lepton flavor-violating observables through radiative corrections. In this talk we discuss and show that these impacts can be significant in the Next-to-Minimal Supersymmetric extension of the Standard Model (NMSSM) including additionally six leptonic singlet superfields.

Presenter: Dao Thi Nhung

I.10 – Invited, VCTP-47

A renormalization group improvement for thermally resummed effective potential

Koichi Funakubo (1), Eibun Senaha (2)

(1) Saga University; (2) Van Lang University

Effective potential is a standard tool to analyze thermal phase transitions. It is known that perturbative expansion at zero temperature breaks down at high temperature due to infrared divergence. To cure this problem, thermal resummation is indispensable. However, the renormalization group (RG) invariance that is present at zero temperature is lost by such a thermal resummation. In this talk, I will begin by showing the RG non-invariance of resummed effective potential in phi-4 theory up to the 2-loop order, and then propose a scheme in which RG invariance holds order by order in resummed perturbation theory. As an example of first-order phase transition, we consider an extension of the phi-4 theory. Our numerical analysis shows that renormalization scale dependences in our scheme could get milder significantly than those in the MS-bar scheme at 1-loop level, while at the 2-loop level the difference between the two schemes are less pronounced as long as couplings are moderate in magnitude.

Presenter: Senaha Eibun

I.11 – Invited, VCTP-47

No-go theorem for inflation in Ricci-inverse gravity

Tuan Q. Do

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Recent, a very novel fourth-order gravity model called the Ricci-inverse gravity has been proposed as a promising approach to the dark energy problem. Motivated by some well-known fourth-order gravity models, e.g., the Starobinsky one, which have been shown to admit inflationary solutions to the early universe, we propose to seek both anisotropic and isotropic inflationary solutions in the Ricci-inverse gravity model. As a result, we are able to figure out analytically the desired ones. However, stability analysis based on the dynamical system method is performed to show that all the obtained inflationary solutions turn out to be unstable unexpectedly. This result therefore forms a no-go theorem for inflation in the Ricci-inverse gravity.

Presenter: Do Quoc Tuan

O.1 – Oral, VCTP-47

The possibility of discovering CPT violation with T2K-II, NOvA-II and JUNO

T. V. Ngoc (1,2), S. Cao (1), N. T. Hong Van (3), P. T. Quyen (1,2)

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The CPT symmetry which is the combination of charge conjugation C, parity inversion P,

and time reversal T, predicts that particle and its antiparticle must have the same mass and lifetime. Neutrino oscillation experiments can precisely measure the mass squared differences ($\Delta m^2_{21}, \Delta m^2_{31}$) and mixing angles ($\theta_{12}, \theta_{13}, \theta_{23}$) of neutrinos and antineutrinos. They therefore can be the best tools for testing CPT invariance. In this talk, we will present the possibility to discover CPT violation with the synergy of T2K-II, NOvA-II and JUNO experiments. The combination of the three experiments will be able to exclude CPT invariance at 3σ C. L. It also can improve the bound on $|\Delta m^2_{31} - \Delta \overline{m}^2_{31}|$ to the world best value ever, $8.3 \times 10^{-5} eV^2$ at 3σ C. L. which is about one order better in magnitude compared to the current value analyzed by neutrino oscillation experiments ($2.5 \times 10^{-4} eV^2$). We also show how the sensitivity depends on true values of the oscillation parameters.

Presenter: Tran Van Ngoc

O.2 – Oral, VCTP-47

Novel effects of the W-boson mass shift in the 3-3-1 model

Duong Van Loi and Phung Van Dong

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The recent precision measurement of the W boson mass reveals an exciting hint for the new physics as of the 3-3-1 model. In this work, we indicate that the 3-3-1 model itself contains distinct sources that cause the W-mass deviation, as measured, such as the tree-level Z-Z' mixing, the tree-level W-Y and Z-Z'-X mixings, as well as the non-degenerate gauge vector (X, Y) and new Higgs doublets. We point out that the gauge vector doublet negligibly contributes to this mass shift, whereas the rest of the effects with tree-level mixings governed by Z-Z' and new Higgs doublets are significant.

Presenter: Duong Van Loi

O.3 – Oral, VCTP-47

Exploration of new equiatomic quaternary Heusler compounds for spintronic applications

Hoang Duc Quang (1), J Guerrero-Sanchez (2), R Ponce-Pérez (2), J. F Rivas-Silva (3), Gregorio H Cocoletzi (3), DM Hoat (4,5)

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Managing electron spin as an additional degree of freedom, besides its charge, leads to the emergence of new physics and formation of new disciplinary called spintronics or spin-based electronics. In the last year, spintronics have rapidly developed in both technological applications and fundamental science, whose expansion has been estimated to be beyond Moore's law. However, the search of new materials for spintronic applications is still a great challenge to optimize the devices functionality. In this work, we present the results of first-principles calculations of two new equiatomic Heusler compounds, namely MnVZrP and CoCrRhSi. As a first

step, the structure design and stability are performed. Electronic and magnetic calculations indicate the ferromagnetic semiconductor and half-metallic natures of the materials, respectively, whose magnetic properties are produced mainly by 3d transition metals. These features suggest the studied quaternaries as prospective candidates for spintronic applications to generate spin current by either spin-filtering or spin injection.

Presenter: Do Minh Hoat

O.4 – Oral, VCTP-47

Cutler-Mott relation and Wiedemann-Franz law on a weak link between two charged Kondo circuits

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We revisit a model describing Seebeck effect on a weak link between two charge Kondo circuits, which has been proposed in the [Phys. Rev. B 97, 085403 (2018)]. We calculate the thermoelectric coefficients in the perturbation theory assuming smallness of the reflection amplitudes of the quantum point contacts. We focus on the linear response equations in three different scenarios as: Fermi liquid vs Fermi liquid, Fermi liquid vs non-Fermi liquid, non-Fermi liquid vs non-Fermi liquid. The oscillations of the thermoelectric coefficients as functions of the gate voltage of each quantum dot are analysed in both Fermi liquid and non-Fermi liquid regimes. We discuss the deviation of thermopower from the value obtained by Cutler-Mott relation and Lorenz ratio from unity. It opens possible experimental realizations of the model to observe the signatures of the non-Fermi liquid behaviour in the thermoelectric transport measurements.

Presenter: Nguyen Thi Kim Thanh

O.5 – Oral, VCTP-47

Extracting terahertz time domain using high-order harmonic generation

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Used to be a gap in electromagnetic spectrum, terahertz (THz) radiation overcame the limits in generation, and being deploited strongly for many applications. As the results, the waveform of THz radiation, i.e. the temporal electric field, plays an important role. In common, the THz waveform is probed by time-domain spectroscopy (TDS). Based on the pump-probe idea, many current methods for THz-TDS treat THz wave as the pump, and the probe can be either a THz or an infrared pulse. Remarkably, all of these methods use lattices as the interacting environment, which may lead to some unexpected effects, such as, phonon absorption, over-rotation, and so on. For this reason, gas is a potential candidate.

In this report, we propose a method to extract the time domain using the high-order harmonic generation (HHG) emitted by the atoms in a combination of an infrared intense laser pulse and a THz pulse. HHG can be simply understood as the emission of photons with frequency of a multiple number of incident laser's frequency. On the contrary to the symmetric laser-target system, whose HHG contains only odd harmonics, the HHG of this system adds the even ones due to the symmetry breaking caused by the THz pulse. It suggests utilizing the even harmonics, in particular, the even-to-odd ratio (the ratio between intensities of even harmonics and the adjacent odd one) to probe the electric field of the THz pulse.

To achieve this goal, we generate HHG by numerically solving the time-dependent Schrödinger equation of atoms in the combined infrared and THz laser pulses. Investigating comprehensively the HHG from different targets and laser pulses, we find out an universal one-to-one dependence of the even-to-odd ratio on the THz's electric field. The analytical expression describing this universal law is performed by the quantum orbit theory. Finally, we use the even-to-odd ratio as a tool to extract the THz time domain. The accuracy and validation of the method is also discussed in detail.

Presenter: Trieu Doan An

O.6 – Oral, VCTP-47

The soft parameter of attractive Coulomb potential in nonsequential double ionization process

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The nonsequential double ionization process is considered using the classical ensemble model. In this model, the choice of soft parameter of attractive Coulomb potential is essitial for avoiding autoionization while maintaining the physical issue of the problems. In the study, we propose a comprehensive procedure to determine the appropriate value of this parameter based on two conditions: ensuring the positive kinetic energy of two electrons and preventing the atom from autoionization. The procedure is illustrated for several noble gas atoms such as Ar, He, Ne, Kr and Xe.

Presenter: Truong Dang Hoai Thu

O.7 – Oral, VCTP-47

The neutrino masses and theirs effects on the Higgs sector of the Next-toTwo Higgs Doublet Model including Inverse Seesaw mechanism

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The Higgs mechanism is the spirit of the Standard Model that generates particle masses. That is the reason why checking the Higgs potential is an important goal in experiments. Although

the couplings of Higgs boson with SM particles have been measured and are consistent with the Standard Model, the Higgs potential has not yet confirmed experimentally. The shape of this potential is govern by a parameter λ, that drives the strength of the Higgs boson self-couplings. It can be determined experimetally through a measurement of Higgs pair production. Currently, its value is still far away from the required accuracy and therefore allows new physics effects.

In this talk, we report on our computation of trilinear Higgs couplings at the one-loop level in the CP-conserving Next-to-Two Higgs Doublet Model including Inverse Seesaw Mechanism by using the Feynman-diagrammatic approach. The Inverse Seesaw Mechanism introduces heavy neutrinos that can give a large contribution to trilinear Higgs couplings. We discuss renormalization schemes used for the Higgs sector to cancel UV divergences. The Feynman rule is generated by SARAH, the amplitude calculated by FeynArt and FormCalc, and we use LoopTools for the computation of loop integrals. We have taken into account constrains from the Higgs data by using HiggsBounds and HiggsSignals, and from neutrino oscillation data to find the available parameter space. We found that loop effects can be of order 30%.

Presenter: Le Truong My Hau

O.8 – Oral, VCTP-47

Unparticle effects at the MUonE experiment

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In this paper, we investigate the effects of unparticles on the muon-electron elastic scattering at the MUonE experiment. Four types of unparticles in consideration are scalar, pseudo-scalar, vector, and axial-vector unparticles. The new physics model depends on two free parameters for each type of unparticle. The muon g-2 measurement and others (e.g. mono-photon, mono-Z searches) impose constraints on those parameters. Using these constraints we study the effects of unparticles in the MUonE experiment.

Presenter: Le Van Dung

O.9 – Oral, VCTP-47

Correlation between energy band transition and optical absorption spectrum in bilayer armchair graphene nanoribbons

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By utilizing atomistic tight-binding description and the gradient approximation, we studied the correlation between absorption spectra and electronic structures of bilayer and single-layer armchair nanoribbons (BL-AGNRs and SL-AGNRs) without and with external electric fields. The alternations of peak structure, gap size, and charge distribution for three groups 3p, 3p+1, and 3p+2 are examined extensively. The remarkable results are: (i) the position and the height of the 1st peaks in the 3p and 3p+1 groups are found to vary as a function of the number of

dimer lines, while those in the 3p+2 group remain unchanged for BL-AGNRs and vanish in the region [0, 0.4t0] for SL-AGNRs; (ii) with the increase of potentials Vt, the red-shift and lowering in the height of the 1st ¬peaks occur for the 3p and 3p+1 groups, meanwhile, addition peaks in the opposite direction are observed for 3p+2 due to the bandgap opening; (iii) the vertical field has a strong impact in modulating the peak structure, meanwhile the transverse field only show its influence on the peak height, especially in the 3p group. Our outcomes provide a more comprehensive understanding of the important role of external electric fields on the optical transition in single-layer and bilayer graphene nanoribbons, and unveil potential applications of these structures in optoelectronics.

Presenter: Nguyen Lam Thuy Duong

O.10 – Oral, VCTP-47

Halogenation effects in silicene and silicene nanoribbons: A DFT study

Duy Khanh Nguyen

High-performance computing laboratory (HPC Lab), Information Technology Center, Thu Dau Mot University, Binh Duong Province, Vietnam

In this talk, I will systematically present the various halogenation effects in structural, electronic, and magnetic properties of 2D silicene and 1D silicene nanoribbons, in which the halogen adatoms-enriched essential properties are fully identified under the complete DFT theoretical framework, including the cohesive energies, optimal structural parameters, phonon band structures, atom-and orbital-dominated electronic band structures, atom- and orbital-projected density of states (DOSs), spatial charge density distributions, charge density difference, magnetic moments, and spin density distributions. For 2D silicene systems, the double-side and single-side halogen effects are fully included in the calculations, whereas the former belongs to the concentration-depended finite gap semiconductors or p-type metals, while the latter display the valence energy bands with/without spin-splitting intersecting with the Fermi level. For 1D armchair silicene nanoribbons (ASiNR), the semiconducting behavior of the pristine system becomes the p-type metallic or semiconducting behaviors under the various halogen concentrations. For zigzag silicene nanoribbons (ZSiNR), the anti-ferromagnetic configuration of pristine ZSiNR transforms into the ferromagnetic one under the single adatom adsorption. Especially, under the double adatom adsorptions, whether the anti-ferromagnetic configuration becomes ferromagnetic or nonmagnetic ones that strongly depends on the adatom distributions across the zigzag edges. The ferromagnetic-nonmagnetic transition of the halogen-adsorbed ZSiNR is found at the critical concentration of 25%. The diverse structural, electronic and magnetic properties of halogenated silicene and silicene nanoribbons are very potential for a wide range of applications in high-performance electronic and spintronic devices.

Presenter: Nguyen Duy Khanh

O.11 – Oral, VCTP-47

Bilayer armchair graphene nanoribbons under the effect of combining vacancy and external electric fields

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In this work, we aim to investigate the electronic structure of bilayer armchair graphene nanoribbons (BL-AGNRs) 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. The results illustrate that the band gaps of BL-AGNRs can be modified by the two factors above. Due to the missing of a single C atom, the energy gap was divided into two almost symmetrical gaps around the Fermi level. Besides, the gap in groups 3p and 3p+1 are narrowed, whereas the opposite trend is true for class 3p+2. Moreover, the various mono-vacancy positions cause the different DOS peaks in energy bands. 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 type and the magnitude of electric fields. This work thus unveils some important conditions for controlling the gap as well as the electronic properties of BL-AGNRs.

Presenter: Nguyen Thi Kim Quyen

O.12 – Oral, VCTP-47

Coulomb divergence in (d,p) reactions based on the Faddeev-Alt-Grassberger-Sandhas equation

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The Faddeev-Alt-Grassberger-Sandhas (FAGS) equation is the most performance formalism to describe the (d,p) reactions since it can exactly and simultaneously treat the elastic, inelastic, transfer, and breakup reactions. However, for the last 60 years, the Coulomb divergence is the most severe barrier which prevents the application of FAGS in the few-body physics context. In this talk, we will describe our efforts in solving the Coulomb divergence in the direct elastic scattering of the (d,p) reaction using the FAGS at low energy.

Presenter: Trần Viết Nhân Hào

O.13 – Oral, VCTP-47

Spin symmetry energy and equation of state of spin-polarized neutron star matter

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The equation of state (EOS) of spin-polarized nuclear matter (NM) is studied within the Hartree-Fock (HF) formalism using the realistic density-dependent nucleon-nucleon interaction. The present HF study shows a strong correlation between the spin symmetry energy and nuclear symmetry energy over the whole range of baryon densities. The important contribution of the spin symmetry energy to the EOS of the spin-polarized NM is found to be comparable with that of the nuclear symmetry energy to the EOS of the isospin-polarized or asymmetric (neutron-rich) NM. Based on the HF energy density, the EOS of the spin-polarized (β-stable) npeμ matter is obtained for the determination of the macroscopic properties of neutron stars (NS). A realistic density dependence of the spin-polarized fraction has been suggested to explore the

impact of the spin symmetry energy on the gravitational mass M and radius R, as well as the tidal deformability of NS. Based on the empirical constrains inferred from a coherent Bayesian analysis of gravitational wave signals of the NS merger GW170817 and the observed masses of the heaviest pulsars, the present study shows the strong impact of the spin symmetry energy W , nuclear symmetry energy S, and nuclear incompressibility K on the EOS of nucleonic matter in magnetar.

Presenter: Ngo Hai Tan

O.14 – Oral, VCTP-47

On the anisotropic constant-roll inflation for the Dirac-Born-Infeld model

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We extend an anisotropic inflation model under the so-called constant-roll condition for a canonical scalar field to that for the Dirac-Born-Infeld scalar field – a string theoretic motivated model in which the canonical kinetic term, $-\frac{1}{2}\partial^\mu\phi\partial_\mu\phi$, is replaced by the non-canonical one, $f^{-1}(\phi)\left[1-\sqrt{1+f(\phi)\partial^\mu\phi\partial_\mu\phi}\right]$. As a result, we find a set of consistent formalisms for the potential $V(\phi)$, a gauge kinetic function $h(\phi)$ in an unusual coupling between scalar and vector fields, $h^2(\phi)F_{\mu\nu}F^{\mu\nu}$, and the function $f(\phi)$, which give us the corresponding anisotropic inflationary solutions. Furthermore, we show that these new solutions are consistent with the canonical case and turn out to be stable via numerical calculations.

Presenter: Nguyen Hoang Duy

O.15 – Oral, VCTP-47

A novel k-Gauss-Bonnet power-law inflation model

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We present a novel inflation model in a framework of the Einstein-scalar-Gauss-Bonnet gravity, where the Gauss-Bonnet topological invariant is allowed to non-minimally couple to the kinetic term of scalar field in the absence of the potential. Remarkably, this model gives an exact power-law solution in a framework of the isotropic and homogeneous universe, which is proved to be stable during the inflationary phase by using the dynamical system method. More interestingly, this model is shown to be free of a gradient instability in tensor perturbations.

Presenter: Pham Manh Tuyen

O.16 – Oral, VCTP-47

A method for retrieving asymmetricity of polar molecule from high harmonic generation

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High-order harmonic generation (HHG) is a highly non-linear optical phenomenon that can be observed when material interacts with an ultrashort intense laser pulse. HHG contains structural and dynamical information of atoms and molecules. Therefore, HHG is a powerful tool to probe the structure of atoms and molecules; and microscopic dynamics of electron and nuclei.

The HHG emission can be understood by the semiclassical three-step model [1]. Accordingly, after propagating in an external electric field, the tunneling electron recombines into the parent ion, leading to the generation of the attosecond bursts with half-cycle time-spacing. For symmetric laser-target systems, generated attosecond bursts are identical (except a π change). Considering the asymmetry system, specifically polar molecule in a multicycle laser pulse, attosecond bursts from two opposite sides are distinguished, both amplitude and phase. Therefore, this microscopic information reflects the asymmetry of polar molecules and becomes attractive to be investigated. Especially, the phase difference between two adjacent attosecond bursts in a train has been extracted from experiments in 2012 [2], in which the phase difference is extracted from the experimental even-to-odd harmonic ratio and the calculated amplitude ratio of the two adjacent attosecond bursts. This ratio is computed from the ionization rate and amplitude of recombination dipole whose accuracy strongly depends on the approximated theory level.

In this work, firstly, we prove that the amplitude ratio and phase difference are inherent properties of polar molecules. We have tested their stability when changing the laser's parameter. We found that the intensity imbalance and the phase difference is almost unchanged with various laser's parameter. Then, we propose a general method to probe the intensity imbalance and the phase difference between two consecutive attosecond bursts from measured HHG data only. In particular, from measured HHG intensity and phase, one can construct the time-frequency spectrogram and directly retrieve the amplitude ratio and phase difference between adjacent attosecond bursts. Using the "numerical experimental" HHG data, we also check the validation of the method. The results show that the method works with high accuracy. Using the "numerical experimental" HHG data, we also check the validation of the method. The results show that the method works with high accuracy.

[1] M. Lewenstein, P. Balcou, M. Y. Ivanov, A. L'Huillier, and P. B. Corkum, Phys. Rev.A, vol. 49, 2117, 1994. [2] E. Frumker et al., Phys. Rev. Lett, vol. 109, 233904, 2012.

Presenter: Nguyen Huynh Kim Ngan

O.17 – Oral, VCTP-47

Generation of dynamic stark-induced degenerate vibronic state by two shift up non-resonant lasers

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In the past it was commonly understood 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 by that the unidirectional π-electron rotation can be created even

in low symmetry aromatic ring molecules using the two linearly polarized lasers with a relative phase [1]. The key point is to create a degenerate electronic state of two quasi-degenerate electronic excited states by applying two non-resonant lasers. Here, vibrational degrees of freedom were not taken into account. In our recent work [2] we have taken into account the nuclear vibrational effects on the unidirectional π-electron rotation in the adiabatic approximation, where a weak coupling model of two electronic states with a few vibrational states is adopted [2], where the two lowest vibronic states in two electronic excited states were set to be degenerate by two lasers (Dynamic Stark induced-Degenerate vibronic state-DSIDVS). Here vibrational states in the electronic excited state 1 are shifted up by the laser a, and the lowest vibrational state in the electronic excited state 2 is shifted down by the laser b, whereas the other vibrational states in the electronic excited state 2 are shifted up by the laser b. Such opposite behaviours in the level shift of the vibronic states in the electronic excited state 2 make it complicate to describe the behaviours of dynamic Stark-induced vibronic states. In this work we propose an alternative method using the two non-resonant shift-up lasers to avoid the complication mentioned above.

[1] H. Mineo, M. Yamaki, G.S. Kim, Y. Teranishi, and Y. Fujimura, Phys. Chem. Chem. Phys. 18, 26786-26795 (2016).

[2] H. Mineo, N.L. Phan, D.K. La and Y. Fujimura, J. Phys. Chem. A 125, 1476-1489 (2021).

Presenter: Ho Quang Huy

O.18 – Oral, VCTP-47

Investigating the inverse Klein tunneling effect in binary waveguide arrays

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Waveguide array (WAs) is 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) - another peculiar fundamental quantum relativistic effect - 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]. The potential step must be sufficiently steep for KT to be observed [8]; i.e., it must occur at a very narrow region comparable or shorter than the Compton wavelength. In this presentation, we show results that we investigated the inverse KT in BWAs. For observing KT in BWAs, one launches an incident beam belonging to the positive branch (or electron branch) of the dispersion relation so that it hits the potential step and generates the transmitted beam belonging to the negative branch (or positron branch). Inversely, to observe the inverse KT effect, we now propose to launch an incident beam belonging to the negative branch which hits the inverse potential step and generates the transmitted beam belonging to the positive branch. In this talk, we want to achieve two goals: (i) we show the analytical formulas for the inverse KT effect in two cases: discrete model and continuous model,

and (ii) we verify these theoretical results for the inverse KT in BWAs by comparing them with the results obtained by the beam propagation method.

REFERENCES

[1] D. N. Christodoulides, F. Lederer, and Y. Silberberg, Nature (London) 424, 817 (2003). [2] D. N. Christodoulides and R. I. Joseph, Opt. Lett. 13, 794 (1988). [3] Tr. X. Tran and F. Biancalana, Phys. Rev. Lett. 110, 113903 (2013). [4] S. Longhi, Phys. Rev. B 81, 075102 (2010). [5] F. Dreisow, R. Keil, A. Tünnermann, S. Nolte, S. Longhi, and A. Szameit, Europhys. Lett. 97, 10008 (2012). [6] O. Klein, Z. Phys. 53, 157 (1929). [7] H. Nitta, T. Kudo, and H. Minowa, Am. J. Phys. 67, 966 (1999). [8] F. Sauter, Z. Phys. 69, 742 (1931)

Presenter: Trần Công Minh

O.19 – Oral, VCTP-47

Construction molecular potential using machine learning

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Theoretical simulation of physical and theoretical phenomena is an essential way to understand their nature and examine experimental observation. The prerequisite task for theoretical simulation is constructing a potential model for molecules, and then solving its Time-Independent Schrödinger Equation (TISE) to get the expected values that are needed to be consistent with experiments. Various methods have been developed for constructing potential model – including the Single Active Electron model with a soft-Coulomb pseudo-potential governed by a set of parameters [1], [2]. For complex molecules, finding a large number of parameters that need to satisfy many outcome conditions by traditional statistical learning faces to challenge due to the limit of computational resources. Besides, solving the TISE is also a costly and time-consuming process. Concurrently, the emergence of machine learning with advanced artificial models capabilities to overcome these difficulties. In this report, we apply machine learning to solving two-fold goals: The first one is re-constructing the soft-Coulomb pseudo-potential of HCN molecule with multiple parameters by optimizing in a way that the energies and permanent dipoles of different molecular orbitals converge to the experimental values. For doing this task, we apply two machine learning algorithms - Neural Network (NN) and Light Gradient Boosting Machine (LGBM) - to predict potential parameters, then combine both predictions to make the final predictions with another algorithm - Random Forest. Similarly, the second one is to solve the inverse problem. We use NN to build surrogate models which solve the TISE to determine rapidly the energies and permanent dipoles based on potential parameters. Both works have fruitful results. The Mean Absolute Percent Error (MAPE) of most paraments in the first task is less than 0.5%. And the Symmetry Mean Absolute Percent Error (sMAPE) of most energies value in the second task is less than 1%. However, the sMAPE of the permanent dipoles is high for some states – this is still in the improvement process.

[1] M. Peters, T. T. Nguyen-Dang, E. Charron, A. Keller, and O. Atabek, "Laser-induced electron diffraction: A tool for molecular orbital imaging," Phys. Rev. A, vol. 85, no. 5, p. 53417, May 2012, doi: 10.1103/PhysRevA.85.053417. [2] C. I. Blaga et al., "Imaging ultrafast molecular dynamics with laser-induced electron diffraction," Nature, vol. 483, no. 7388, pp. 194–197, 2012, doi: 10.1038/nature10820.

Presenter: Hoàng Trọng Đại Dương

P.1 – Poster, VCTP-47

Field- and anisotropy-induced critical points and specific heat of XYZ ferromagnetic chain with single-ion anisotropy

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Hue university of Education

The functional integral method is used to study critical properties, field- and anisotropy induced critical points, energy spectra of spin waves and specific heat of a one-dimensional XYZ ferromagnet with the added single-ion anisotropy in a skew magnetic field. Quantization axis is defined to lie in the yz-plane. Depending on the strength of the anisotropy and the magnetic field, a finite-temperature critical line found, which ends in quantum critical point, exists for the spin chain. Moreover, a double-peak structure of specific heat in temperature dependence which is found for XYZ chain depending on the strength of the anisotropy and on the magnetic field, manifesting competition of magnetic orders in different directions.

Presenter: Phạm Hương Thảo

P.2 – Poster, VCTP-47

Multiple returns in continuum harmonics of asymmetric molecules in multicycle lasers

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A wide range of continuum harmonics is essential for generating attosecond pulse trains. It is commonly used longer-wavelength lasers to push the cutoff to a higher order. However, this also enhances the contribution of higher-order returns (HOR) in a harmonic spectrum, consequently, potentially affecting the lower bound of the continuum range. It is desired to understand how multiple returns affect the harmonic-spectrum structure and their response to different laser parameters. This report presents the manifestation of multiple returns in the high-order harmonic spectra from CO molecules by numerically solving the time-dependent Schroedinger equation within the single-active electron approximation. Based on the time-frequency analysis [1] and the classical simulation [2], we justify the multiple returns effect and the periodicity of the harmonic spectrum of CO. Furthermore, the time-frequency spectra show that the high-order returns not only are asymmetric regarding the molecular rotation of 180 degrees but also correlate with the first-order returns. Finally, we figure out that one can control the contribution of HOR by breaking the laser symmetry in an appropriate way.

References [1] Y.-l. Sheu, L.-Y. Hsu, H.-t. Wu, P.-C. Li, and S.-I. Chu, AIP Advances 4, 117138 (2014). [2] P. B. Corkum, Phys. Rev. Lett. 71, 1994 (1993).

Presenter: Le Thi Cam Tu

P.3 – Poster, VCTP-47

Retrieval of structural information of monolayer transition-metal dichalcogenides from exciton energy spectra

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We report a new procedure for retrieving the structural information, such as the reduced exciton mass, screening length, and dielectric constant of monolayer transition-metal dichalcogenides (TMDs), from the experimental exciton energy spectra. The main idea is based on the fact that the Keldysh potential describes well the interaction between electron and hole. This interaction potential differs from the Coulomb potential at short distances due to the low-dimensional effect that makes it very sensitive to the structural parameters. We consider these structural quantities as free parameters and choose their appropriate values to fit the calculated exciton energy spectrum of 1s, 2s, 3s, and 4s states for the recently published experimental data [1] - [3].

For our purpose, we have built a computing program for exciton energies of monolayer TMDs in the magnetic field with high precision up to 15 decimal places by the Feranchuk-Komarov (FK) operator method [4]. The FK operator method combined with the Levi-Civita transformation allows purely algebraic calculations with the creation and annihilation operators. One advantage of this work is to present the Keldysh potential through the Laplace transform that makes all the matrix elements calculated analytically. The exact analytic expressions of these matrix elements reduce computational resources significantly. Therefore, we can apply the method for ground and highly excited states. Especially, the program can be used for the states with non-zero magnetic quantum number m, better than the previous program working only for s states.

[1] A. V. Stier, N. P. Wilson, K. A. Velizhanin, J. Kono, X. Xu, and S. A. Crooker, Magnetooptics of Exciton Rydberg States in a Monolayer Semiconductor, PRL 120 (2018) 057405.

[2] M. Goryca et al., Revealing exciton masses and dielectric properties of monolayer semiconductors with high magnetic fields, Nat. Commun. 10 (2019) 4172.

[3] J. Have, N. M. R. Peres, and T. G. Pedersen, Excitonic magneto-optics in monolayer transition metal dichalcogenides: From nanoribbons to two-dimensional response, PRB 100 (2019) 1–10.

[4] I. Feranchuk, A. Ivanov, Van-Hoang Le, A. Ulyanenkov, Non-perturbative Description of Quantum Systems, Springer, 2015.

Presenter: Ly Duy-Nhat

P.4 – Poster, VCTP-47

Structural diversity and optoelectronic properties of chemical modification pentagonal quantum dots

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A first-principle study of the structural diversity and optoelectronic properties of the small pentagraphene (PG) quantum dots (PGQDs) has been performed. The stability and optoelectronic properties of the PGQDs are investigated under the effect of chemical modifications. PGQDs are edge functionalized by non-metallic atoms (H, P, Si, O) such as identical edge termination (H-PGQD, P-PGQD, Si-PGQD, O-PGQD) and alternate edge termination (H-O-PGQD, Si-O-PGQD, H-P-PGQD). Further, H-PGQDs are also doped and co-doped with B and P atoms. All studied structures are stable with strong electronic quantization and exhibit semiconducting or metal properties depending on the termination and doping elements and their site. Absorption peaks in the visible region were not observed for hydrogen passivation PGQDs. However, some absorption peaks appear in this region for edge-passivated. In addition, there are changes in the electronic properties of PGQD samples containing impurities B, P, or BP also give a shift in the peak of the spectrum to the visible region from the ultraviolet region of the corresponding pure sample. This is because of various hybridization effects in PG and PGQDs with edge passivation and atom doping. The enhanced reactivity, and controllable electronic properties of edge passivation, and doping make PGQDs ideal for new nanodevice applications.

Presenter: Nguyen Thi My Hang

P.5 – Poster, VCTP-47

Effect of confined optical phonons on photo-stimulated Ettingshausen effect in rectangular quantum wires with a perpendicular field.

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We apply the quantum kinetic equation method to investigate the influence of confined optical phonons (confined OP) on the photo-stimulated Ettingshausen effect in rectangular quantum wires (RQW) subjected to a perpendicular magnetic field. We considered the case where the confined electrons-confined OP scattering is the dominant mechanism. Analytical expressions for the kinetic tensors, the Ettingshausen and the temperature difference (ΔTy) are obtained. The Ettingshausen confined (EC) is a function of external fields, the temperature of the system, especially the quantum numbers m1 and m2 characterizing confined OP. The numerical results are numerically evaluated and discussed for the GaAs/AlGaAs RQW .The magnitude of the resonance peaks in the case confined OP has been risen about 3,6 times compared to the case unconfined OP, found when examining the dependence of the EC on the magnetic field. Besides, the dependence of the temperature difference (ΔTy) on the cyclotron energy was also found. It is shown that ΔTy has been changed by about 45K. These results were indicated that the EC and the temperature difference ΔTy were influenced by the confinement optical phonons. These results are important for further researches and can be helped to complete the theory of the thermo-magnetoelectric effects in low dimensional system. Keywords: Confined optical phonon, the quantum Ettingshausen effect, rectangular quantum wires, quantum kinetic equation, photo-stimulated effect.

Presenter: Cao Thị Vi Ba

P.6 – Poster, VCTP-47

Optimization of TiN-based ultraflexible materials for photothermal and solar harvesting applications

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We propose a theoretical model to investigate photothermal heating of ultraflexible metamaterials, which are obtained by randomly mixing TiN nanoparticles in PDMS. Due to the plasmonic properties of TiN nanoparticles, incident light can be perfectly absorbed in a broadband range (300-2500 nm) to generate heat within these metamaterials. Under irradiation of an 808 nm near-infrared laser with different intensities, our predicted temperature rises as a function of time agree well with recent experimental data. For a given laser intensity, the temperature rise varies non-monotonically with the concentration of TiN nanoparticles. Increasing the TiN concentration leads to a decrease in the heating process since the thermal conductivity grows. A small TiN concentration significantly reduces the absorbed energy and, thus, the system is less heated. When we apply this model to solar heating, we find that the temperature rise is no longer non-monotonic, and the heating efficiency is much lower than in the laser case. Our studies would provide good guidance for future experimental studies on the photothermal heating of broadband perfect absorbers.

Presenter: Do Thi Nga

P.7 – Poster, VCTP-47

Theoretical study of photostimulated Nernst effect in cylindrical quantum wires

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The photostimulated Nernst effect in cylindrical quantum wires under the influence of confined optical phonons (confined OP) is studied by using the quantum kinetic equation method. We presume that the confined electrons-confined OP scattering is essential. The analytical expression for the kinetic tensors and the Nernst coefficient (NC) have been determined, they are functions of external fields, the temperature of the system, the radius of the wires, especially the quantum number m1 and m2 describe confined OP. The theoretical results are numerically estimated and discussed for the cylindrical quantum wires (CQW) of GaAs/AlGaAs. The inter-subband magnetophonon resonance condition was demonstrated when analyzing the dependence NC on the photon energy. The confined OP has increased the NC about 2.3 times compared with the unconfined OP case. This change was also found when investigating the effect of the magnetic field on the NC. Besides, at the high temperature, the NC which increased considerably was achieved when examining the dependence of NC on the temperature. All numerical results indicated that the NC was affected by the confined OP and the presence of EMW. In addition, these results obtained in this work are different in comparison with the bulk semiconductors case.

Presenter: Nguyen Thu Huong

P.8 – Poster, VCTP-47

Nested logistic map model: An application in immune system research

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The primitive logistic map model is considered an effective phenomenological theoretical tool in many interdisciplinary research fields. In recent reports, in last years of 2020 and 2021, the logistic map model has been extended and modified to study the variability of virus infection rates within and between communities with different medical and immunological conditions during the Covid-19 pandemic. In the framework of the generalization of the logistic map model, a nested logistic map model with two dynamic or more variables that respond to each other's change is proposed to investigate the role of the immune system in the development of the virus, as determined through viral load tests. Numerical results for the nested logistic map model have shown different scenarios in the correlations between viral development and the response of the immune system in the body.

Presenter: Nguyen Van Hoa

P.9 – Poster, VCTP-47

The influence of partial boundary scattering on Seebeck coefficient oscillation in granular thermoelectric thin films

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We investigate the Seebeck coefficient oscillations in thermoelectric thin films with rectangular grain structure. Within a relaxation time approximation, the Seebeck coefficient is shown to increase due to inelastic scattering on the grain boundaries along the temperature gradient direction but it decreases with partial scattering on the thickness boundary direction. Quantum effect is distinctly revealed in the variance of oscillation amplitude of the Seebeck coefficient with reducing the grain size. The effective mass of carriers and the Fermi energy of the film are key parameters determining both the amplitude and period of the oscillations.

Presenter: Bach Giang

P.10 – Poster, VCTP-47

Proton entropy excess and possible signature of pairing reentrance in hot nuclei

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In this work, we investigated the entropy excess caused by one proton (the so-called proton entropy excess) for several pairs of medium and heavy mass nuclei using the available nuclear level density data. Results obtained show that the proton entropy excess as a function of excitation energy $E*$ can be well described by the recent microscopic calculations based on the exact pairing plus independent-particle model at finite temperature (EP+IPM). It is also observed that the proton entropy excess is ∼0.1–0.5 kB for the spherical nuclei and ∼1.0–1.2 kB for the deformed ones. These values are notably smaller than those obtained from the neutron entropy excess (∼1.3–2.0 kB). This is due to the effect of Coulomb interaction as well as the proton single-particle level densities, which is less than the neutron ones. In particular, we observed a peak-like structure in the proton entropy excess at low $E* < 1$ MeV. This structure is possibly associated with the pairing reentrance phenomenon caused by the weakening of blocking effect in odd nuclei at low temperature as explained by the EP+IPM. This peak-like structure is more pronounced in the spherical nuclei than in the deformed isotopes [1].

Reference:

[1] Balaram Dey, Srijit Bhattacharya, Deepak Pandit, N. Dinh Dang, N. Ngoc Anh, L. Tan Phuc, and N. Quang Hung, Phys. Lett. B 819, 136445 (2021).

Presenter: Nguyen Quang Hung

P.11 – Poster, VCTP-47

The new entanglement criterion for two-mode systems and application

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This paper proposes a new entanglement criterion for two-mode systems based on a phase difference operator with Hermite form and a particle difference operator. This new criterion is applied to quantify the entanglement degree of the pair coherent states (PCS) and the photon added and subtracted two-mode pair coherence states (PAASTMPCS). The results show that these states are strongly entangled, and their entanglement degree increases rapidly to the maximum when the coherence amplitude increases up a few units. Besides, adding and subtracting photons make the entanglement degree of PAASTMPCS improve significantly, especially in the region with small coherence amplitude. We also compared the results of applying the new entanglement criterion and the linear Entropy criterion for the states mentioned above and found many similarities between these two criteria. This criterion is created from the phase difference operator and the particle difference operator, so it has great potential to apply to the families of states where the phase parameter plays an important role.

Presenter: Ho Sy Chuong

P.12 – Poster, VCTP-47

Mass-dependent binding energies of trions in parabolic quantum dots

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The binding energies of quasi-particles in semiconductor nano-structures play a very important role in the design of electronic devices. In this paper, by using the Hartree-Fock method, we investigate the binding energy of trions in two-dimensional quantum dots with a parabolic confinement potential in dependence on the effective masses of electrons and holes. We obtained interesting results showing that there are bound-to-unbound or unbound-to-bound transitions of trions that depend on the effective mass ratio between electrons and holes.

Presenter: Nguyen Que Huong

P.13 – Poster, VCTP-47

Zn-doped configurations in Germanene nanoribbons in electric field: A DFT study

Hoang Van Ngoc

Thu Dau Mot University

Germanene nanoribbons (GeNRs) are one-dimensional materials with a narrow band gap, doping another element into GeNRs helps to create new materials. Electric fields also have an important role in controlling the electromagnetic properties of materials. The doping of Zn into GeNRs in a constant external electric field aims to create materials with larger bandgap as well as to create new materials. By using DFT theory and VASP software, five Zn-doped configurations in electric field are studied here. The configurations are optimized, durable and stable. Configuration 1-1 proved to be superior in terms of stability, doping replaces two Zn atoms and six Zn atoms for an opened band gap of about 0.5eV, with this band gap fully applicable. in a field transistor at room temperature.

Presenter: Hoang Van Ngoc

P.14 – Poster, VCTP-47

Magneto-optical responses in silicene

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We study the optical response properties of silicene in the presence of a non-uniform magnetic field. Analytical expressions for the longitudinal $\chi_{xx}(\omega)$ and Hall $\chi_{yx}(\omega)$ susceptibilities are derived from the equation of motion method. The $\chi_{xx}(\omega)$ and $\chi_{yx}(\omega)$ are evaluated as functions of photon energy for both undoped and doped systems for different values of electron densities, temperatures, magnetic field penetration, and magnetic fields. At $T = 0$, the intra-band transitions induce only one peak while the inter-band ones cause a series of peaks that show oscillations with photon energy. The electron density is one of the main factors controlling the threshold energy in the doped regime.

Presenter: Huynh V. Phuc

P.15 – Poster, VCTP-47

A first-principles investigation of methanal gas absorption on WS2 monolayer

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In this work, we investigate the adsorption mechanism of methanal (the simplest aldehyde) molecule on the monolayer WS2 surface using the density functional theory (DFT). To characterize the adsorption of this gas molecule and the WS2 substrate, we adopt DFT simulations with taking into account the van de Waals (vdW) interactions. The global minimum energy configuration and binding energy of methanal adsorbed WS2 were determined using the Computational DFT-based Nanoscope tool in order to image the binding possibilities of gas molecule adsorbed on the surface of WS2. The adsorption energy profiles were calculated by employing five non-emperical vdW functionals, namely revPBE-vdW, optPBE-vdW, vdW-DF2, optB88, and optB86b. The detailed discussion on the interaction between methanal gas molecule and the WS2 substrate in terms of charge transfer, altered density of states and band structure, substrate deformation, and a series of calculated parameters such as adsorption distance, response length, recovery time, work function, bond length and angle will be given. We found that the adsorption of methanal on the WS2 substrate is physical with an adsorption energy of 224 meV. Upon adsorption, the bandgap is reduced up to 21 meV, and the 0.18 electron transfer from the substrate to gas.

Presenter: Huy Tran Quang

P.16 – Poster, VCTP-47

Exciton behaviors in monolayer WSe_2 under isotropic strain

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We present a density functionals study of the exciton behaviors under isotropic strain in monolayer WSe_2. Firstly, the formation of optical and momentum excitons is explored by analyzing the spin projected band structure of the strainless material. Then, the essential effects such as the reduction of the bandgap and the change in the dispersion degree of the energy extrema near the gap caused by strain are revealed. We found that the modification in the electronic structure due to the tensile strain enhances the direct transitions and hinders indirect transitions of electrons from the valence band to the conduction band. Therefore, tensile may lead to an additional appearance of optical excitons and a disappearance of momentum excitons. The change of the electronic structure caused by the compression enhances the indirect transitions and counteracts direct transitions, resulting in the additional appearance of the momentum

excitons and disappearance of optical excitons. These findings can provide a possible path to manipulate the excitons in monolayer transition metal dichalcogenide materials upon isotropic strain.

Presenter: Tran Thị Nhan

P.17 – Poster, VCTP-47

One-loop contribution for H → ZZ* → Z f f in Standard Models

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One-loop contributions for H → ZZ* → Z f f in Standard Models are presented in this talk. Analytic formulas are expressed in terms of Passarino-Veltman functions in the standard notations of LoopTools. Hence, the decay rates can be computed numerically by using this package. Differential decay rates with respect to transverse momentum of Z boson, invariant mass of fermion pair are discussed in this work.

Presenter: Trần Trí Dũng

P.18 – Poster, VCTP-47

The characteristic frequency equation and the semi-empirical formula for the coupling strength in cantilever array

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In this work, we figure out a characteristic frequency equation of the T-shaped and overhang-shaped cantilevers. We consider the overhang lengths and widths that change the resonant frequencies and mode shapes. The obtained results reveal the number of optimum values of the frequencies corresponding to the mode shapes. Furthermore, a semi-empirical formula for the coupling strength of cantilevers in an array is proposed. It shows a good agreement between the theoretical model and the values obtained in experiments by other studies.

Presenter: Le Tri Dat

P.19 – Poster, VCTP-47

Role of thermal quantities in framework of nuclear pairing correlation

Le Tan Phuc

Institute of Fundamental and Applied Sciences, Duy Tan University

Thermodynamics play an important role in many fields of physics, especially, in the phase transition of matter. In the framework of nuclear pairing correlation, the thermal quantities such as heat capacity and entropy are the signature of the transition between normal state and superconductivity state. This talk is a brief report of the role of heat capacity and entropy in nuclear pairing effect. Some recently results, which are obtained during the investigation of pairing re-entrance effect at finite temperature, are shown.

Presenter: Le Tan Phuc

P.20 – Poster, VCTP-47

Grafting Methionine on 1F1 Antibody Increases the Broad-Activity on HA Structural-Conserved Residues of H1, H2, and H3 Influenza A Viruses

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A high level of mutation enables the influenza A virus (IAV) to resist antibiotics treatment. A portion of the structure of hemagglutinin (HA), a protein of IAV responsible for cellular entry is assumed to be well-conserved to maintain its role, while the structure tends to be more conserved than sequence. We aimed to increase the breadth of activity of the complementarity-determining regions (CDR) of antibodies known to target H1 subtype of IAV so that the CDR can target H2 and H3 subtypes as well. The design entailed grafting onto the CDR with a hotspot amino acid that formed favorable contact with the conserved residues on the HA surface identified based on structural alignment. The contact was evaluated using molecular docking, a method employing empirical functions to calculate the change of free energy upon molecular binding. Methionine amino acid was scored best when it is interacting with Tyrosine, Arginine, and Glutamic acid on HA. The methionine-grafted CDR fragment were found to be to form in silico contact with a structurally conserved region across H1, H2, and H3 HA. The binding site lies at the boundary between HA1 and HA2 domains, spreading across different monomers, suggesting a new target for designing broad-spectrum antibody and vaccine. This research presents an affordable method to enhance the spectrum of CDR from known antibodies based on hotspot grafting assisted by molecular docking.

Presenter: Lê Thanh Hòa

P.21 – Poster, VCTP-47

Electron transport through experimentally controllable parabolic bubbles on graphene nanoribbons

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We present a theoretical study of electron transport properties through experimentally controllable graphene nanobubbles [1] employing a tight-binding model and the non-equilibrium Green's function formalism. Sharp conductance peaks are observed at low energy region which signifies the emergence of quasi-bound states caused by pseudomagnetic field in the strained nanobubbles. Analysis based on local density of states reveals the nature of electron transmission at peak energies. Our results also show that the emergence of quasi-bound states and its role in electron transport depend on both strain strength and bubble size: when the strain or size of the bubble increases, more quasi-bound states emerge and resonant tunnelling assisted by these quasi-bound states becomes dominant.

[1] P. Jia, W. Chen, J. Qiao, M. Zhang, X. Zheng, Z. Xue, R. Liang, C. Tian, L. He, Z. Di et al., Nat. Commun. 10 (2019) 1.

Presenter: Nguyen Mai Chung

P.22 – Poster, VCTP-47

Toward multi-target drug therapeutic of Chronic obstructive pulmonary disease: In silico study of Ergosterol using molecular docking, molecular dynamics simulation and binding free energy

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It is doubtful that single-target drugs have limited efficacy against complex diseases in which the pathogenesis is dependent on a set of biochemical events and several receptors. Multi-target drugs offer the possibility to overcome the issues as they are defined as a compound or a group of compounds acting through multiple targets of a relevant disease, hence, providing bioactivity. Multi-targeting in herbal medicine is understood as the interplay of multiple components in plant extract and has become an excellent resource for multi-target drug discovery. In this research, we study the possibility of discovering multi-target drugs for chronic obstructive pulmonary disease (COPD) from natural products. The mechanisms of COPD are well studied, and their disease targets are systematically classified into groups such as bronchodilators, inflammatory modulators, proteases, antioxidants, kinase inhibitors, phosphodiesterase, and others. Ergosterol, a compound available in both Vietnamese and Chinese traditional herbal medicine, was used in COPD treatment and proved its efficacy. However, their mechanisms of action are still unclear. This research applied molecular docking, molecular dynamics, and binding free energy in understanding the interaction between ergosterol and COPD disease targets. Our simulation suggested that ergosterol had potential interactions with different target groups and is a promising candidate for further multi-target drug development.

Presenter: Do Tuan

P.23 – Poster, VCTP-47

Islands in regular black strings

Tran Ngoc Hung, Cao Hoang Nam, Doan Minh Luong

Phenikaa University

We apply the quantum extremal surface prescription to calculate the Page curve for five and higher dimensional regular black strings. The results in the configuration without island show that the entanglement entropy of the Hawking radiation grows over time and becomes infinite at late times. Taking into account of one island configuration which emerges at the late times of the evaporation, the entanglement entropy becomes saturated and is equal to twice of the Bekenstein-Hawking entropy of the black string. We find that the boundary of island is outside but near the event horizon. The result with the island configuration is consistent with the finiteness of the entanglement entropy of the Hawking radiation for an eternal black string.

Presenter: Tran Ngoc Hung

P.24 – Poster, VCTP-47

Edge states in a model of magnetic topological insulators

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We construct a model for magnetic topological insulators and study the edge states in its nanoribbon. The model is a combination of the Kane-Mele and the double exchange models on a honeycomb lattice. We apply an inhomogeneous dynamical mean field model to the proposed model. We find different edge states in the paramagnetic topological, antiferromagnetic topological, antiferromagnetic topologically trivial and antiferromagnetic half-topological insulating states.

Presenter: Nguyễn Hồng Sơn

P.25 – Poster, VCTP-47

Divacancy effects on the electronic properties of zigzag buckling silicene nanoribbons

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In this study, we used the tight-binding calculation and Green's function methodology to investigate the band structure as well as the density of states (DOS) of zigzag buckling silicene nanoribbons (ZBSiNRs) in divacancy (DV). In particularly, the number and position of vacancies are going to demonstrate in this paper. Furthermore, the external electric fields are utilized as a function of the gap size in both two cases with and without vacancies. The results illustrate that the material still exhibits the metallic nature of ZBSiNRs under the impact of divacancy. However, the flatband state has been transformed to the upward-sloping band. This is the special result in the energy bands of this material. In addition, we realized that the electronic properties of ZBSiNRs are strongly depends on the number and position of vacancies. Specially, the peak intensity at the Fermi level in DOS is strongly increasing, which leads to increment more electronic transmission channels under the presence of external electric fields. 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.26 – Poster, VCTP-47

Feature-rich structural and electronic properties of halogen-functionalized germanene nanoribbons: A DFT study

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Structural and electronic properties of halogen (F, Cl, Br, I, and At)-functionalized armchair germanene nanoribbons (AGeNR) are investigated using the density functional theory (DFT) method. The first-principles quantities are fully developed to determine the studying properties, including the functionalized energies, optimal structural parameters, atom- and orbital-decomposed electronic band structures and density of states, charge density distribution, and charge density difference. The halogen-functionalized structures achieve good stability that is determined by the calculated functionalized energies. The pristine AGeNR presents a direct bandgap of 0.44 eV that becomes 0.76 eV, 0.73 eV, 0.51 eV, 0.16 eV, and semimetal in the F-AGeNR, Cl-AGeNR, Br-AGeNR, I-AGeNR, and At-AGeNR, respectively. The bandgap-diversified mechanism is due to the termination of free-standing π bonds and complex orbital hybridization in halogen-Ge bonds. The domination in subbands occurs at deeper energies starting from F-AGeNR, Cl-AGeNR, Br-AGeNR, I-AGeNR, and At-AGeNR that is owing to shorter and longer halogen-Ge bond lengths. Under halogen functionalizations, electrons are transferred from Ge atoms to halogen adatoms that create free holes in the functionalized systems that can be regarded as the p-type semiconductors/semimetals. The diverse structural and electronic properties of halogen-functionalized AGeNR show that the p-type 1D systems will be very potential for various electronic applications. Keywords: DFT calculations, halogen functionalization, electronic band structures, electronic density of states, electron transfer, p-type semiconductors, and electronic applications.

Presenter: Vo Van On

P.27 – Poster, VCTP-47

Optical refraction and absorption spectra in perturbed monolayer PbBiI

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We investigate the optical properties of a noncentrosymmetric quantum spin Hall insulator in the presence of electric and magnetic fields. We employ the Kubo formula to engineer the optical redshift and blueshift phenomena through the interplay between the bulk gap, the Rashba-like gap, and the external fields. Intriguingly, for a range of electric (magnetic) fields, the refracted and absorbed lights exhibit direct (indirect) interband optical transitions. Accordingly, for a critical electric field, optical refraction and absorption spectrum decreases gradually and becomes constant, respectively. While for a critical magnetic field, step-like jumps appear in the optical

coefficients. All these findings are discussed in the context of symmetry breaking.

Presenter: Le Thi Thu Phuong

P.28 – Poster, VCTP-47

Effect of gate voltage on the anisotropic optical transitions of β_{12}-borophene

Hoang Van Ngoc (1), Bui Dinh Hoi (2)

(1) Thu Dau Mot University; (2) University of Education, Hue University

The honeycomb lattice of β_{12}-borophene has two types of triplet and Dirac fermions with different momenta. The coexistence of these fermions engenders anisotropic optical responses. The main goal of this work is to engineer the effect of electrostatic gating on such responses. We numerically calculate an effective optical conductivity tensor to address the effect of gate voltage on the blueshift (along the x-direction) and redshift (along the y-direction) spectra through multi-interband transitions. We also find a blueshift spectrum for the Hall conductivity. Further, we investigate the role of partial optical interband transitions on the total effective transitions. The findings here can be considered for practical optoelectronic applications.

Presenter: Bui Dinh Hoi

P.29 – Poster, VCTP-47

Energy of hydrogen atom in excited states induced by static electric field

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As atom/molecule is exposed to an external electric field, it can be ionized. Besides, the energy of the atomic/molecule system is altered due to the influence of the atom/molecule – electric field interaction. The hydrogen atom is one of the simplest system to explore and is in current attention. In this paper, we numerically calculate the dependency of the energy of the hydrogen atom in arbitrarily excited states, including all degenerating states. The results are validated using second order perturbation theory.

Presenter: Pham Quang Huy

P.30 – Poster, VCTP-47

The interaction between Bose – Einstein Condensate fluid and fixed potential wall

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In this study, the imaginary-time, split-operator methods combining with Fast Fourier Transform

are used to numerically simulate the Bose – Einstein Condensate (BEC) dynamics by solving Gross – Pitaevskii equation. the BEC is considered in harmonic trap as the density profile fit with Thomas – Fermi distribution. We take into account the sliding effect of two BEC components in opposite directions. Thus, we are alble to investigate the pattern of Kelvin – Helmholtz instability at the boundary surface between two components. As the two BEC components slide on each other with the same direction and velocity, they are considered to interact with a mountain-like Gaussian potial wall. This effect procedues the Lee wave phenomena.

Presenter: Pham Nguyen Thanh Vinh

P.31 – Poster, VCTP-47

Applying first principle to study the structure, electrical and optical properties of Sc adsorbed ASiNRs

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In this project, we studying the structural, electrical, and magnetic properties of adsorption of Sc on Armchair Silicene nanoribbons (ASiNRs) in three steps. The first, the hollow position is chosen from four positions bridge, hollow, valley, and top because adsorbed energy is the largest. The second, with the bond length, Si-Si is 2.36 AA, and adsorption energy – 4.18 AA is the best structure state. Finally, the high Sc atom on the surface ASiNRs 1.25 AA was optimized. The result after Sc adsorbed ASiNRs, new materials are semi-metal, they have a magnetic property as candidates for the spintronic device, the electronic device in future. Keywords: adsorbed Sc, adsorption chemical, semi-metal

Presenter: Nguyen Thanh Tung

P.32 – Poster, VCTP-47

One-loop contributions to the decay processes $H \to f f^{-} \gamma$ in beyond the Standard Model.

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General one-loop contributions to the decay processes $H \to f f^{-} \gamma$ and its applications are presented in this paper. We consider all possible contributions of the additional heavy vector gauge bosons, heavy fermions, and charged (also neutral) scalar particles propagating in Feynman loop diagrams. Therefore, analytic results are valid in a wide class of models beyond the Standard Model. Analytic formulas for the form factors are expressed in terms of Passarino-Veltman functions in the standard notations of LoopTools. Hence, the decay rates can be evaluated numerically by using this package. The computations are then applied to the cases of the Standard Model, $U(1)B - L$ extension of the Standard Model as well as Two Higgs Doublet Model. Phe-

nomenological results for all the above models are studied. We observe that the effects of new physics are sizable contributions and these can be probed at future colliders.

Presenter: Phan Hong Khiem

P.33 – Poster, VCTP-47

Ferromagnetic Magnon in Monolayer Honeycomb Spin Lattice in The Application of Transverse Field

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We investigate electronic band structures of ferromagnetic magnon in the monolayer honeycomb spin lattice using the anisotropic XZ-Heisenberg model in the transverse field (TF). It is shown that the nature of this magnetic phase transition is the spin reorientation (SR) transition in the presence of TF. Besides, two magnon branches exist in the temperature region above the SR temperature. The transverse field decreases or increases the spin wave intensity in the temperature region below or above the SR temperature, respectively and the gap of the zero momentum of the lower magnon branch ϵ_0^- closes at the critical transverse field Ω_0C of the quantum phase transition at zero temperature. By fitting our model with the zero momentum magnon mode experimentally observed in ferromagnetic monolayer CrI3, the derived exchange parameters agree well with the DFT calculation.

Presenter: Nguyễn Từ Niệm

P.34 – Poster, VCTP-47

Entanglement, nonlocality, quantum teleportation of two-mode non-Gaussian states with multiphoton quantum catalysis

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In this paper, we introduce new two-mode non-Gaussian entangled states, called multiphoton catalytic pair coherent states (MCPCSs), based on the study of multiphoton quantum catalysis on two-mode non-Gaussian states, which are the pair coherent states (PCSs). By investigating linear entropy, Einstein-Podolsky-Rosen (EPR) correlation and EPR steering, it is shown that these properties in the new states can be enhanced compared with the PCSs by increasing the coherent parameter amplitude $|\xi|$. In the small regions of $|\xi|$ and in transmission coefficients space, the enhanced regions of the degree of entanglement are enlarged with increasing number of catalytic photons, whereas in contrast to the EPR correlation and the EPR steering. Using the MCPCSs as entanglement sources to teleport a coherent state via the Braunstein and Kimble protocol, we calculate the average fidelity F of the teleportation process. The investigated results show that the average fidelity is enhanced in the large regions of the transmission coefficients as small valuesof $|\xi|$. In particular, for zero-photon catalysis, F is improved in the case of $|\xi|$ high.

Presenter: Tran Quang Dat

P.35 – Poster, VCTP-47

Study of the thermodynamic properties of BaTiO3 perovskite by the statistical moment method with improved interatomic potential.

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(1) Hung Vuong University and VNU University of Science; (2) VNU University of Education

We study the thermodynamic properties of cubic BaTiO3 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 BaTiO3, are obtained. The potential with the partial charge model and functions of Demontis and Pedone is used to calculate the numerical thermodynamic quantities of BaTiO3 from room temperature up to high temperature. The numerical results of the thermodynamic quantities of BaTiO3 by the statistical moment method up to high temperatures and pressures 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 BaTiO3 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.36 – Poster, VCTP-47

Open Kondo circuit as a detector for electron-electron interactions in a Luttinger Liquid

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We investigate the effects of the electron-electron (e-e) interactions on quantum transport in a one dimensional system. We demonstrate it by considering the model in which a quantum dot is sandwiched between two finite quantum wires or quantum point contacts. We show that the open quantum dot can be used as an e-e interaction detector: the temperature scaling of the electric conductance is affected by the interaction in the electron gas through the Luttinger parameter g. Two limits: $L \ll a$ and $L \gg a$ are considered with L and a are the size of the Luttinger liquid wires and the quantum dot, correspondingly. We also discuss the influence of e-e interactions on the non-Fermi liquid behavior of the conductance at the two channel Kondo fixed point. Besides, our results bring back the electron interaction independent dc conductance e^2/h in the finite length quantum wires.

Presenter: Nguyễn Hồng Quang

P.37 – Poster, VCTP-47

Stability, geometrical and electronic structures of the mixed aluminum – scandium clusters AlxScy, with x + y = 13

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Geometrical and electronic structures of 13-atom clusters AlxScy, with x + y = 13, as well as their thermodynamic stabilities were investigated using DFT calculations. The results reveal that both anionic and neutral isomers of AlxScy favor the icosahedral shapes in which Sc atoms locate at exohedral positions of icosahedral cage to maximize the stronger bonds Al-Al and Sc-Al instead of the weaker one Sc-Sc. NBO analyses were applied to examine the electronic configurations and rationalize the high electron spin multiplicities of the clusters having more than three Sc atoms. The obtained results proved that the spatial orbitals of the SOMOs are the molecular orbitals belonging to the irreducible representations of the symmetry point group of the clusters studied. The evaluation of the average binding energy showed that the thermodynamic stability of AlxScy clusters alters insignificantly as y goes from 0 to 7 and then decrease steadily with y in the 7 – 13 range. Moreover, increasing the number of Sc atoms also causes the electron affinity of the AlxScy clusters to be reduced and thus they loss the halogen characteristics in comparison with the pure Al13.

Presenter: Nguyen Minh Tam

P.38 – Poster, VCTP-47

Phase diagram of the half-filled disordered Hubbard model at finite temperature

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Institute of Physics, VAST

We study metal-insulator phase diagram in the half-filled disordered Hubbard model at finite temperatures. By means of dynamical mean field theory with an impurity solver of the equation of motion method, we calculate the averaged local density of states at the Fermi level and the site occupation as a function of the site energy at different temperatures. The paramagnetic phase diagram at finite temperature is constructed numerically and compared with the one at T = 0.

Presenter: Hoang Anh Tuan

P.39 – Poster, VCTP-47

First-principles insights into the Janus group III monochalcogenides

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Two-dimensional Janus structures with vertical intrinsic electric fields exhibit many interesting physical properties that are not possible with symmetric materials [1]. In this study, we design and predict the structural, electronic, transport, and optical properties of twodimensional Janus GaInXO (X = S, Se, Te) monolayers by using first-principles calculations [2]. The stability of

all six possible configurations of GaInXO was examined through the analysis of their phonon spectra. It is found that, except for the OGaInTe monolayer, all the other configurations are dynamically stable. Further, the mechanical stability has been also investigated via calculations for the elastic constants. Depending on the stacking configuration, GaInXO can be either semiconductor (with a direct or indirect band gap) or metallic. Interestingly, the carrier mobilities of the investigated systems are found to be highly directional isotropic; however, the mobility of electrons is much higher than that of holes, suggesting that these monolayers can be potential materials for applications in nanoscale electronics. Finally, strong optical absorption in a wide light region extending from the infrared to the ultraviolet region is also predicted in the Janus GaInXO depending on its stacking configuration. The findings not only get insights into the fundamental properties of the Janus materials based on group III monochalcogenide monolayers but also suggest them as potential candidates for applications in the next-generation optoelectronic nanodevices.

Reference: [1] Nguyen N. Hieu, Huynh V. Phuc, A. I. Kartamyshev, and Tuan V. Vu, Phys. Rev. B 105 (2022) 075402. [2] Tuan V. Vu, Vo T. T. Vi, Huynh V. Phuc, A. I. Kartamyshev, and Nguyen N. Hieu, Phys. Rev. B 104 (2021) 115410.

Presenter: Nguyen Ngoc Hieu

P.40 – Poster, VCTP-47

Structural, electronic properties of pentagonal $PdSe_2$ nanoribbons: a first-principles calculations

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A first-principle study of the structural diversity and optoelectronic properties of the various edge pentagonal $PdSe_2$ nanoribbons has been performed. In 2017, scientists successfully synthesized the few-layered $PdSe_2$ (FL-$PdSe_2$) from bulk crystals, a pentagonal 2D layered noble transition metal dichalcogenide with a puckered morphology that is air-stable. They confirmed that the field-effect transistors made from the FL- $PdSe_2$ display tunable ambipolar charge carrier conduction with a high electron field-effect mobility, indicating the promise of this anisotropic, air-stable, pentagonal 2D material for electronic devices. This work investigated the structural and electronic properties of p-$PdSe_2$ nanoribbons (p-$PdSe_2$NRs) using density functional theory (DFT). Herein, we propose a series of new p-$PdSe_2$NRs by cutting p-$PdSe_2$ sheets. Our first-principles calculations show that p-$PdSe_2$NRs are energetically stable, and a semiconductor excludes sawtooth-sawtooth p-$PdSe_2$NR. These findings provide valuable insight into a novel material structure in low-dimensional material systems for potential nanoelectronics.

Presenter: Nguyen Thanh Tien

P.41 – Poster, VCTP-47

Conductivity in the disordered Hubbard model at half-filling

Nguyen Thi Hai Yen, Hoang Anh Tuan

Institute of Physics

In this work, the optical and dc conductivity for half-filled disordered Hubbard model for various cases in the weak and the intermediate interaction regimes are calculated within the typical

medium theory. The influence of random potential and temperature on the optical and dc conductivity in the model is investigated. It is shown that in some cases the disorder can weaken the correlation effect, moves the system away from Mott transition and decreases resistivity of the system.

Presenter: Nguyen Thi Hai Yen

P.42 – Poster, VCTP-47

Neutrino mass spectrum with the present neutrino data

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Neutrino oscillations discovered by Super-Kamiokande 1998, Sudbury Neutrino Observatory 2001, and others resulted in the existence of neutrino mass. This quantum mechanic phenomenon is beyond the description of the Standard Model and being explored for unearthing the mysteries in the particle physics. Neutrino mass is exceptionally small and physicists are unsure of its origin. Also, the neutrino mass spectrum is not precisely established yet. The neutrino mass is known to us from four sources: neutrino oscillation, cosmology, beta decay, and the search for neutrino-less double beta decay. In this work, we use a neutrino mass model in which neutrinos are assumed to be Majorana particles to reconstruct neutrino mass using the current constraints from all of these sources. The results show that, unlike quarks and charged leptons, the neutrino's reconstructive mass matrix does not follow any obvious hierarchy. This matrix is also shown to be dependent on the value of the CP-violation phase in the leptonic mixing matrix. As a result, precise measurement of the CP-violation is also critical for casting light on the neutrino mass model.

Presenter: Phan To Quyen

P.43 – Poster, VCTP-47

Magnon spectrum of the spin-1 J1 –J2 antiferromagnetic Heisenbeberg model on a triangular lattice

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We study the spin-1 antiferromagnetic Heisenberg model on a triangular lattice with nearest J1 and next-nearest-neighbor J2 exchange interactions. The auxiliary fermionic representation of the spin operators within a functional integral formalism with an imaginary Lagrange multiplier is employed to retain an exact constraint of single particle occupancy. Reprensentating the classical ground state by Luttinger-Tisza procedure one may consider the fluctuation contributions to the free energy of the system in the entire range of the coupling parameters. We derived the magnon spectrum in one-loop approximation. The obtained magnon spectrum is compared with the result of the Green functions Mori's projection operator technique.

Presenter: Nguyễn Văn Hinh

P.44 – Poster, VCTP-47

A molecular dynamics simulations of penta silicene anoribbons affected by size, edge and pressure

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We present molecular dynamics (MD) simulations of melting of penta silicene nanoribbons (penta SiNNRBs) from the crystal state under the non-periodic boundary conditions with/without pressure. We used four models which differ in the number of atoms and type of edge. Zigzag edge containing 3034 and 6347 atoms Si, sawtooth edge containing 3106 and 6049 atoms arranged a penta structure with the buckling d = 1.49 AA and the minimum interatomic distance equal 2.23AA, maximum equal 2.36 AA. We heated a model from temperature 50 K to 3000K to get a liquid state, then we cooled the models to 300 K. We use the same melting and cooling rate, $\gamma = 2 \times 10^{11}$ K/s. We also studied the effects of pressure on the models by compressing the model at 2000 K, 1500 K and 1000 K. Structure and thermodynamics properties upon melting are studied and presented, such as the temperature dependence of total energy per atoms, radial distribution functions (RDF), coordination number, bond and angle distribution, interatomic distance between an atoms in models. 2D visualization of atomic configurations at certain temperature is presented by VMD software. Melting of penta SiNNRBs from the crystal state has been affected by size and type of edge. Beside, pressure is a factor that affects the structure formed at 300 K.

Presenter: Trang Như Hải

P.45 – Poster, VCTP-47

Size, type boundary and pressure effect on silicene nanoribbons by molecular dynamics simulation

Nguyen Thi Bich Doanh (1), Nguyen Thi Ngoc Tuyen (1), Truong Quoc Tuan (1), Ngo Hai Yen (1), Ong Kim Le (2), Huynh Anh Huy (3)

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Structures and properties of thermodynamics in silicene nanoribbons (SiNNRBs) are carried by molecular dynamics simulation (MDs) under non-periodic boundary conditions. We used a crystal SiNNRBs models with armchair boundary containing 3000, 6000 and 10000 atoms, and zigzag boundary containing 3096, 6052 and 9976 atoms is arranged a honeycomb structure with the low-buckling of and a bond length Si-Si equal . All models are heated to a temperature much higher melting point with melting rate , then cooled to room temperature with cooling rate , we also compress model contain 10000 atoms at three temperature 2000 K, 1500 K and 1000 K to investigate Evolution of structure and thermodynamics properties upon melting, cooling and compress is studied and discussed, such as radial distribution functions, temperature dependence of total energy per atoms, coordination number, bond and angle distribution, interatomic distance between Si-Si. 2D visualization of atomic configurations are also presented. Melting and cooling of SiNNRBs from the crystal state has been effected by size of model and boundary condition, pressure also effect on phase change of silicene to penta or tetra silicene.

Presenter: Nguyễn Thị Bích Doanh

P.46 – Poster, VCTP-47

Entanglement and quantum teleportation with nonlinear charge pair cat states

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In this paper, we investigate the entanglement degree of the nonlinear charge pair cat states using the linear entropy criterion. It is shown that these states are entangled and their entanglement degree depends on the nonlinear functions f(n). We have used these states for teleportation of a coherent state in two different measurements at the sender by using joint measurements of the quadrature amplitude and joint measurements of the photon number sum and phase difference. The investigated results show that the even nonlinear charge pair cat states are more suitable for teleportation in the way of the quadrature amplitude measurements. However, in the joint measurement of the photon number sum and phase difference, these states are suitable for the teleportation process in the small amplitude of the coherent state. Keywords: nonlinear charge pair cat states; entanglement degree; quantum teleportation

Presenter: Dang Huu Dinh

P.47 – Poster, VCTP-47

Investigation of pairing phase transition in some excited meadium nuclei

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The pairing phase transition in some excited meadium nuclei are investigated by using extrapolating the experimental nuclear level densities (NLDs). Those data below the neutron binding energy B_n are combined with the back-shifted Fermi-gas (BSFG) model for the energy above B_n and up to about 120 MeV. The energy-dependent level density parameter in the BSFG format is suggested to be used to obtain the best fit to the NLDs. The S-shape observed in the heat capacities of both even and odd isotopes give a precise description of the pairing phase transition in these isotopes.

Presenter: Le Thi Quynh Huong

P.48 – Poster, VCTP-47

Extracting asymmetricity of polar molecular from high order harmonic generation: effect of partial orientation

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Probing molecular asymmetricity is crucial to understanding the nature of polar molecules. Recently, we proposed a method to probe the intrinsic properties, particularly the intensities imbalance and the phase difference of adjacent attosecond bursts from experimental measurements of high-order harmonic generation (HHG) emitted from polar molecules interacting with an intense laser pulse [1]. This method's idea is based on retrieving these quantities directly

from the time-frequency spectrogram constructed by the measured spectral intensity and phase of HHG. The advantage of this method compared with the one given in the previous study [2] is that our method requires measured data only and does not need pre-calculating quantities whose accuracy is strongly dependent on the level of theory. To probe the asymmetricity by HHG, the polar molecular sample must be aligned and oriented before interacting with a probe pulse. However, a perfect orientation and alignment are infeasible even with recent advanced techniques. This report presents an improvement of our method to incorporate the partial orientation of a molecular sample for retrieving the intensity imbalance and phase difference from its HHG. To develop this method, we analytically analyze the time-frequency of a single polar molecule and comparing with the one of a partially oriented sample constructed from HHG measurements. After acquiring the analytical formula, the inference of the intensity imbalance and phase difference of single polar molecular from experimental data of HHG emitted from a partially oriented sample is straightforward. Besides, the effect of the imperfect alignment on the method validation is also discussed. The results show that the improved method works reliably with general HHG experiments.

[1] Kim-Ngan H. Nguyen, Ngoc-Loan Phan, Cam-Tu Le, Dinh-Duy Vu, Van-Hoang Le, 2022, in preparation. [2] E. Frumker, N. Kajumba, J. B. Bertrand, H. J. Wörner, C. T. Hebeisen, P. Hockett, M. Spanner, S. Patchkovskii, G. G. Paulus, D. M. Villeneuve, A. Naumov and P. B. Corkum, Phys. Rev. Lett., 2012, 109, 233904.

Presenter: Phan Ngoc-Loan

P.49 – Poster, VCTP-47

Functional integral approach for the Heisenberg model: beyond one-loop approximation

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We study the Heisenberg model by a functional integral method based on the semionic representation of spin operators, suggested by Popov and Fedotov. The partition function of the spin system is written in term of the functional integral over coherent Grassmann variables with an imaginary chemical potential for excluding non-physical states appeared due to the transformation from spin operators to fermionic ones. We go beyond one-loop approximation taking into account coupling between transverse and longitudinal spin components. The magnon energy is derived and compared with one-loop approximation result. The longitudinal excitation appears and is compared with the result obtained by Feynman method.

Presenter: Pham Thi Thanh Nga

P.50 – Poster, VCTP-47

Quantum teleportation of entangled states via generalized photon-added pair coherent state

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In this paper, we study the quantum teleportation of atomic as well as field states based on the two-photon Jaynes-Cummings model consisting of an effective two-level atom with a two-mode field in the generalized photon-added pair coherent state. By applying the detecting method, we use a given scheme including two two-level atoms and a cavity field to teleport approximately and conditionally an unknown atomic state. Besides, teleporting a state of cavity field to another one with only one atom by using this method is also carried out. In addition, the success probability and fidelity of these teleportation are also considered.

Presenter: Le Thi Hong Thanh

P.51 – Poster, VCTP-47

A first-principles investigation of toxic gases absorption on MoSe2 monolayer

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Here, we study the adsorption of MoSe2 monolayer towards two main harmful gases NH3 and NO2. The density functional theory (DFT) simulations calculations were employed to obtain the adsorption configurations and the adsorption energies of NH3, and NO2 on MoSe2. The van der Waals interactions are taken into account by using five functionals namely revPBE-vdW, optPBE-vdW, optB88, optB86b and vdW-DF2. Using the Computational DFT-based Nanoscope tool, the most stable adsorption configurations and diffusion possibilities of gas molecules on the surface of MoSe2 were determined. The adsorbed molecules influence the electronic behaviour of monolayer MoSe2 and the electric polarity of both the adsorbent and adsorbate. Our findings suggest a possibility of MoSe2 as a potential material for controlled hazardous gas sensing.

Presenter: Luong Thi Theu

P.52 – Poster, VCTP-47

Effects of hydrophobic and electrostatic interactions on the escape of proteins at archaeal and bacterial ribosomal exit tunnels

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We study the escape process of nascent proteins at the ribosome exit tunnels of archaeal Haloarcula marismortui and bacterial Escherichia coli by using combined coarse-grained and atomistic models and molecular dynamics simulations. It is shown that for both types of organisms the electrostatic and hydrophobic interactions of the exit tunnel have similar effects on the escape of small globular proteins. The escape time distribution always maps to a simple diffusion model

in various types of the tunnel model, with and without electrostatic and hydrophobic interactions. An exception is found for the escape of CI2 protein, wherein the hydrophobic interaction of the bacteria exit tunnel significantly slows down the escape process. We also find that the median escape time strongly correlates with the number of hydrophobic residues, N_h, and the net charge, Q, of a protein. Interestingly, the correlation coefficient 0.958 and a combined quantity of $N_h + 5.9Q$ for E.coli (excluding CI2 protein) is quite the same as those for Haloarcula marismortui.

Presenter: Bui Phuong Thuy

P.53 – Poster, VCTP-47

Can DNA form twisted bundles in toroidal condensates?

Nhung T. T. Nguyen and Trinh Xuan Hoang

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Toroidal structures are the most frequently observed morphology of DNA condensates. While the packing of DNAs inside the toroids can be essentially revealed by experiment, it is much less clear about the global conformations adopted by DNAs in the condensates. In this study, we consider a model of toroidal condensate that corresponds to a twisted bundle arrangement of the chain conformation and compare it to other models which are akin to a spool-like and a constant-curvature wrapping, respectively. It is shown that for the toroid energy consisting of a bending energy and a surface energy term, the twisted bundle model always yields optimal conformations of lower energies than the other models. For the ranges of polymer length and surface tension relevant to DNA condensates, the twist number k* of the optimal twisted bundle toroid is found to vary between 0.84 and 1. To find support for the analytical results, we carried out replica-exchange molecular dynamics (REMD) simulations of stiff polymers with self-attraction. Interestingly, the simulations show that twisted bundle toroids can be obtained in the collapse of these polymers. The twisted bundle conformations, however, are limited to relatively short chains due to the polymeric constraint. For longer chains, the viable toroidal conformations appear to be largely spool-like with some disordered parts.

Presenter: Nguyễn Thị Thùy Nhung

P.54 – Poster, VCTP-47

Indentifying the key sites for the thermal stability of glucose-6-phosphate dehydrogenase from a structure-based model

Nhung T. T. Nguyen and Trinh Xuan Hoang

Institute of Physics, Vietnam Academy of Science and Technology

Glucose-6-phosphate dehydrogenase (G6PD) is an enzyme which catalyzes the oxidation of G6P and the reduction of NADP+ to NADPH in the pentose phosphate pathway. The NADPH generation through this metabolic pathway in red blood cells is crucial in protecting the red cells against oxidative damage. The deficiency of G6PD may lead to red blood cell breakdown causing hemolytic anemia. G6PD deficiency is genetically inherited and is known as the most common enzymopathy, affecting 5% of the world population. The activity of G6PD has been shown to correlate with its thermal stability. In this study, we investigate the thermal stability of G6PD by using molecular dynamics simulations with a coarse-grained structure-based model. We identify the key sites defined as the positions in the amino acid sequence that have the largest

contributions to the specific heat of the enzyme. It is shown that a statistically significant fraction of these key sites are linked to point mutations associated with G6PD deficiency.

Presenter: Trinh Xuan Hoang

P.55 – Poster, VCTP-47

Physics implication from a Z_3 symmetry of hadrons

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I show that breaking $B - L$ by one unit of this charge is suitable for neutrino mass generation through an inverse seesaw mechanism, stabilizing a dark matter candidate without supersymmetry, as well as solving the muon anomalous magnetic moment and the W mass deviation via dark field contributions. The new physics is governed by the residual Z_3 symmetry of $B - L$ isomorphic to the center of the color group, instead of the well-studied matter parity.

Presenter: Phung Van Dong

P.56 – Poster, VCTP-47

Investigating the structural features of SRAS-CoV-2 Mpro binding site bound covalent ligands at physiological temperature

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The SARS-CoV-2 pandemic was firstly detected at the end of December 2019 in China, and quickly spread around the world, has been heavy threating global health. Although various COVID-19 vaccines and drugs are approved, developing antiviral drugs and vaccines against COVID-19 virus with high effectiveness is a long-term measure. The SARS-CoV-2 Mpro protein plays important roles in replication and transcription to this viral cycle life, together with three other targets for developing potential drugs treatment to COVID-19 patients. In this research, we investigate the SARS-CoV-2 Mpro binding site bound covalent ligands, 11a and 11b at physiology temperature (310K) using all-atom simulations, then compare to their X-ray experimental structures (at 273K) for understanding the thermodynamic features. We found that conformations of both Mpro proteins and covalent ligands are stable during 500ns of the simulation time. The ligand 11b are more flexible conformation than ligand 11a, meaning that both of them are potential leader compounds for binding to Mpro binding site against SARS-CoV-2, and the covalent ligand 11a has higher binding affinity, as their experiment reported. In addition, the configures of side chains, specially, the catalytic residue H41 and E166, located in the binding sites of Mpro protein are changed a bit in our simulations for easier binding to the ligands and stable structure, while these thermodynamics features are not found in experimental structures. These results are a root for developing candidate drugs against SARS-CoV-2 and other viral strains in the future.

Presenter: Nguyễn Thế Toàn

P.57 – Poster, VCTP-47

Studying the effect of structure on the dynamics in MgSiO4 by a molecular dynamics simulation

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In this paper, the dynamic properties in MgSiO4 liquid are investigated by means of molecular dynamics (MD) simulation. Our model informed that the total radial distribution function is a good agreement experiment and other simulation data. The simulation shows that the structure of MgSiO4 liquid comprises MgOx (x = 3, 4...9) units distributed in Si-O network structure. Mg-O, Si-O linked clusters lend to form a structural heterogeneity. The Mg atom plays the role of both a network-forming element and an element that changes the network structure of silica. Under compression, the fraction of each type of Mg atom changes. This leads to a change in the diffusion coefficient of the Mg atom which diffuses by alone hopping and collective movement. Keywords: MgSiO4 liquid, network structure, diffusion, hopping, collective.

Presenter: Giap Thi Thuy Trang

P.58 – Poster, VCTP-47

H2 physisorption on the internal surface of metal organic framework MOF-74 based materials by ab initio molecular dynamics simulation

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MOF-74 is one of the best H2 physisorptive metal organic frameworks owing to the occurrence of unsaturated metal sites, called open metal sites, which induces strong electrostatic H2 attraction. However, the host – guest binding strength is still needed to be further enhanced for efficient hydrogen storage at ambient conditions. In this work, MOF-74 was modified in various ways including linker functionalization, linker substitution, open metal site fluorination. The H2 adsorption positions on the internal surface of the materials were investigated by ab initio molecular dynamics simulations. The electronic structures were examined to demonstrate the host-guest binding mechanisms. It was shown that using shorter non-aromatic linker can increase the density of strong adsorption sites but the binding strength is slightly reduces by 1.5 kJ/mol due to the absence of aromatic ring. Functionalizing the aromatic linker with -OH, -F, -NH3 functional groups reduces the aromaticity of the ring so that the H2 affinity of the framework reduces. The fluorine atom capping at open metal site shows remarkable H2 adsorption performance. It can adsorb 4 H2 molecules with binding strength larger than all non-open-metal sites in the original framework by 4 kJ/mol.

Presenter: Nguyen Thuy Trang

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Index

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IOP vast

Vietnam Academy of Science and Technology

UNESCO

United Nations Educational, Scientific and Cultural Organization

INTERNATIONAL CENTRE OF PHYSICS
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