Program & Abstracts

41st National Conference
on Theoretical Physics

HỘI NGHỊ VẬT LÝ LÝ THUYẾT TOÀN QUỐC LẦN THỨ 41

Nha Trang
1 – 4 August 2016

Program & Abstracts

41st National Conference on Theoretical Physics

Galina Hotel & Spa
5 Hùng Vương, Lộc Thọ
Nha Trang, Việt Nam

1-4 August 2016

Contents

Welcome Message

It is a great pleasure to welcome you in the *41st National Conference on Theoretical Physics* (NCTP-41) in Nha Trang city.

The NCTP-41 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).

The NCTP-41 is also a branch of the VIII Vietnam National Physics Conference to be organized in 2016.

For over 40 years, the NCTP has been an annual activity of VTPS, and has become the most well-known annual scientific forum dedicated to the dissemination of the latest development in the field of theoretical physics within the country.

Our mission is to foster scientific exchanges between theoretical and computational physicists in Vietnam and worldwide, and to promote a high-standard level of research and education in Vietnam.

Coming to this year conference are nearly 120 participants from more than 30 research and educational institutions in Vietnam. Two invited talks, 22 oral and 79 poster contributions will be presented at the conference.

We wish you enjoy the scientific atmosphere at the conference and have a memorable stay in Nha Trang.

Nguyen Ai Viet
Chair of NCTP-41

Nguyen Ai Viet is with Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST), and he is currently President of the Vietnamese Theoretical Physics Society.

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- Vietnam Academy of Science and Technology (VAST)

General Information

Conference Venue

The NCTP-41 conference takes place in:

Galina Hotel & Spa
5 Hung Vuong, Loc Tho
Nha Trang, Khanh Hoa, Vietnam.

Direction

The conference venue is 35 km from Cam Ranh International Airport (CXR). To get to the conference venue from the airport, participants can either use buses or taxis.

The Cam Ranh - Nha Trang buses cost about VND 70,000 and bring you to the center of Nha Trang city. Tickets can be purchased inside the arrival hall.

Taxis are readily available as you exit the airport. The price for one way trip is VND 250,000 - 300,000 ($12-15).

About Nha Trang

Historically, Nha Trang was known as Kauthara under the Champa before becoming officially Vietnam's territory in 1698. The name Nha Trang was derived from Ya Trang – the name of the

Cái river as referred to by the Cham people, and appeared in various books and maps during the 17th and 18th centuries, including Phủ biên tạp lục (1776) by Lê Quý Đôn.

The city now is still home to the famous Po Nagar Tower built by the Champa. Being a coastal city, Nha Trang is a centre for marine science based at the Nha Trang Oceanography Institute. The Hòn Mun marine protected area, enriched with beautiful coral reef and diverse ecosystems (cover image), is one of four first marine protected areas in the world admitted by the IUCN (International Union for Conservation of Nature).

The Nha Trang Pasteur Institute was established by the French-Swiss bacteriologist Alexandre Yersin who lived in Nha Trang for 50 years until his death in 1943.

Instructions for Speakers

Speakers are requested to be present in their respective session room at least 10 minutes prior to the commencement of the session.

The duration of an invited talk is 30 minutes. This includes 25 minutes for the presentation itself and 5 minutes for Q&A. The duration of a regular presentation is 20 minutes. This includes 17 minutes for presentation itself and 3 minutes for Q&A. We would appreciate it if all presenters can adhere strictly to these time limits.

Speakers should bring their own laptop ready for presentation. Laptop needs to be checked with the projector to be sure it is working before the session starts. No overhead projectors will be made available.

Instructions for Posters

Two poster sessions of the NCTP-41 will be held during 08:30 AM - 10:00 AM in the mornings of 2 August and 3 August, respectively.

Poster should be prepared as one page of size A0 (841 mm x 1189 mm) in portrait (vertical) mode. Please hang your poster on the poster standee with a correct presentation code as given in the abstract book.

At least, the corresponding author of the poster should be present during poster session.

Instructions for Session Chairs

Please be aware of the time frame designated to each presenter, and warn the presenters as follows:

- Invited talk: first warning at 20 minutes, second warning at 25 minutes
- Regular talk: first warning at 15 minutes, second warning at 17 minutes.

Meeting Room

All sessions take place in the conference room on the 2nd floor of Galina Hotel.

Program Timetable

Time	Monday 1 August	Tuesday 2 August	Wednesday 3 August
08:30 – 10:00	Registration Opening (9:00) D. N. Son (I.1) *(Chairs: N. A. Viet)*	Poster Session 1 (P.1 – P.40) *(Chair: D. V. Soa)*	Poster Session 2 (P.41 – P.79) *(Chair: H. A. Tuan)*
10:00 – 10:30	Coffee break		
10:30 – 12:00	N. D. Chinh (O.1) N. T. Dung (O.2) D. D. Long (O.3) N. T. H. Yen (O.4) *(Chair: B. T. Cong)*	T. H. Nam (I.2) D. V. Duc (O.12) N. H. Tung (O.13) D. Q. Tuan (O.14) *(Chair: L. V. Hoang)*	P. N. Hung (O.15) L. D. Nam (O.16) T. T. Thuc (O.17) D. N. Dinh (O.18) *(Chair: D. V. Duc)*
12:00 – 14:00	Lunch time		
14:00 – 15:30	T. T. Duong (O.5) N. D. Huy (O.6) N. V. Duc (O.7) V. T. Tra (O.8) *(Chair: V. N. Tuoc)*	Excursion	N. H. Giang (O.19) T. V. Quang (O.20) V. N. Tuoc (O.21) L. V. Vinh (O.22) *(Chair: P. K. Hung)*
15:30 – 16:00	Coffee break		Coffee break
16:00 – 17:00	N. H. Son (O.9) T. T. Hai (O.10) L. T. C. Tu (O.11) *(Chair: N. T. Thang)*		Closing VTPS Meeting
from 18:00		Gala Dinner	

Lunches

Lunches are provided for conference participants during 1-3 August in the Galina Hotel. Lunch coupons are included in your name badge holder.

Gala Dinner

All participants are invited to Gala Dinner:

BBQ Buffet Menu
Time: 2 August 2016, from 18:00 PM
Place: 2nd Floor, Galina Hotel & Spa.

For your accompanied family members to attend Gala Dinner, please buy tickets (VND 450,000 per person) from the conference secretary on 1 August.

Excursion

Tours around Nha Trang, including those to Hòn Mun and to Khoáng nóng Trăm Trứng, are available in the afternoon of Tuesday, 2 August, at the cost of individuals. Please contact registration desk for tour registration.

VTPS Meeting

A regular meeting of the Vietnamese Theoretical Physics Society (VTPS) will be held right after closing the conference:

Time: 16:10 PM - 17:00 PM, 3 August 2016
Place: 2nd floor, Galina Hotel & Spa.

The meeting program includes announcement and delivery of the VTPS's Young Research Award to Dr. Tran Hoai Nam (Duy Tan University).

Conference Program

Monday, 1 August 2016

08:00 - 09:00 Registration

Opening Session
Chair: Nguyen Ai Viet

09:00 - 09:10 Introduction of delegates

09:10 - 09:25 Welcome Speech by Prof. Acad. Nguyen Van Hieu

09:25 - 09:55 I.1 – Invited
Ab initio study of Pd-skin/Pd3Fe(111) Electrocatalyst for oxygen reduction reaction
Do Son (Ho Chi Minh City University of Technology)

09:55 - 10:00 Photo Session

10:00 - 10:30 Coffee Break

Oral Session 1
Chair: Bach Thanh Cong

10:30 - 10:50 O.1 – Oral
Atom-atom and atom-body dispersion potential in a cylindrical system
Nguyen Dung Chinh (Theoretical Physics Research Group, Faculty of Applied Sciences, Ton Duc Thang University)

10:50 - 11:10 O.2 – Oral
Higher order non-classicalities in the Kerr-like coupler systems
Nguyen Thi Dung (Hong Duc University)

11:10 - 11:30 O.3 – Oral
A study of supersolid phase in square lattice Bose Hubbard model at finite temperature using quantum Monte Carlo simulation
Dang Dinh Long (VNU University of Engineering and Technology)

11:30 - 11:50 O.4 – Oral
Two-component fermions in optical lattice with spatially alternating interactions
Nguyen Thi Hai Yen (Institute of Physics)

12:00 - 14:00 Lunch Break

Oral Session 2
Chair: Vu Ngoc Tuoc

14:00 - 14:20 O.5 – Oral
Strutural organization and network structure of liquid zircon under compression
Tran Thuy Duong (Hanoi University of Science and Technology)

14:20 - 14:40 O.6 – Oral
First-Principles Study on Electronic Structures and Oxygen Vacancy Formation in Strained LaNiO3 Structures
Nguyen Duy Huy (VNU University of Science)

14:40 - 15:00 O.7 – Oral
Grand-canonical Monte-Carlo simulation of salt mixtures and an application to study osmotic pressure of DNA bundle
Nguyen Viet Duc (Faculty of Physics, VNU University of science)

15:00 - 15:20 O.8 – Oral
Modulation of bandgap in armchair bilayer graphene ribbons: a comparison between vertical and transverse fields
Vu Thanh Tra (Can Tho University)

15:30 - 16:00 Coffee Break

Oral Session 3
Chair: Nguyen Toan Thang

16:00 - 16:20 O.9 – Oral
Magnetic and topological transitions in an insulator with doped magnetic impurities
Nguyen Hong Son (Trade Union University)

16:20 - 16:40 O.10 – Oral
The main scattering mechanisms in Single-side modulation doped square quantum wells
Trần Thị Hải (Faculty of Natural Science, Hong Duc University, Thanh Hoa)

16:40 - 17:00 O.11 – Oral
High-order harmonic generation by using single-active electron model potential
Le Thi Cam Tu (Sai Gon University)

Tuesday, 2 August 2016

Poster Session 1
Chair: Dang Van Soa

08:30 - 10:00 P.1 – Poster

Hydrogen storage in MIL-88: Computational study

O My Na (Ho Chi Minh City University of Technology)

08:30 - 10:00 P.2 – Poster

Phonon-assisted cyclotron resonance in MoS2 on polar substrates via two photon absorption process

Huỳnh Vĩnh Phúc (Trường Đại học Đồng Tháp)

08:30 - 10:00 P.3 – Poster

Metal-insulator phase diagram for the fully diagonal disordered Hubbard model at half-filling

Hoang Anh-Tuan (Institute of Physics - VAST)

08:30 - 10:00 P.4 – Poster

Protection of a non-Fermi liquid by spin-orbit interaction

Nguyen Thi Kim Thanh (Institute of Physics, VAST)

08:30 - 10:00 P.5 – Poster

Spontaneous decay rate of a two-level atom in the presence of a multilayered-cylindrical waveguide

Trần Minh Hiến (Viện Vật lý Tp. HCM)

08:30 - 10:00 P.6 – Poster

Electronic properties of monolayer molybdenum disulphide under strain: An ab-initio calculations

Nguyen Ngoc Hieu (Duy Tan University)

08:30 - 10:00 P.7 – Poster

Effects of external electric fields on transmission and Seebeck coefficients in Bilayer Graphene nanoribbons

Nguyen Thi Kim Hue (Can Tho University)

08:30 - 10:00 P.8 – Poster

Some applications using the connection between q-deformed harmonic oscillator and two types of symmetric and asymmetric harmonic potentials

Ngô Gia Vịnh (Bac Ninh Department of Education and Training)

08:30 - 10:00 P.9 – Poster

Derivation of the general formula to describe the Stark shifted energy for Hydrogen atom under the influence of static electric field

Pham Nguyen Thanh Vinh (Ho Chi Minh University of Pedagogy)

08:30 - 10:00 P.10 – Poster

Investigation of thermodynamic and mechanical properties of AlxIn1-xP alloys by Statistical Moment Method

Ho Khac Hieu (Duy Tan University)

08:30 - 10:00 P.11 – Poster

Invariance of probability density functions and transition between Gaussian

and Boltzmann forms of envelope functions problem in the similarity between q-deform harmonic oscillator and Cooper pair
Mẫn Văn Ngữ (Hung Yen Industrial Colleage)

08:30 - 10:00 P.12 – Poster
Quality of joint remote state preparation subjected to noises
Nguyen Van Hop (Department of Physics, Hanoi National University of Education)

08:30 - 10:00 P.13 – Poster
Thermodynamic properties of thin films described by the transverse Ising model
Nguyễn Từ Niệm (VNU University of Science)

08:30 - 10:00 P.14 – Poster
Cooling rate effects on formation of 2D solid with square lattice structure from liquid state
Nguyen To Nga (PetroVietnam University)

08:30 - 10:00 P.15 – Poster
Diffusion of interstitial atoms in interstitial alloys FeSi and FeH with BCC structure under pressure
Nguyễn Thị Hòa (University of Transport and Communications)

08:30 - 10:00 P.16 – Poster
On the mass enhancement of black body background fluctuations
Le Van Xuan (Dong Xuan, Soc Son, Ha Noi, Viet Nam)

08:30 - 10:00 P.17 – Poster
Influence of the Confined Optical Phonon on the Radioelectric Effect in a Cylindrical Quantum Wire in the presence of Laser Radiation
Nguyen Quang Bau (Faculty of Physics, Hanoi University of Science, Vietnam National University)

08:30 - 10:00 P.18 – Poster
Dynamical compactification of extra dimensions on the codimension 2-brane
Do Thi Hong Hai (Department of physics, Hanoi University of Mining and Geology)

08:30 - 10:00 P.19 – Poster
Ideas about building a accelerator driven system (ADS) no target and uses thorium as a nuclear fuel
Tran Minh Tien (Thu Dau Mot University)

08:30 - 10:00 P.20 – Poster
Multiple Component Correlations in Quantum Mixtures of Ultracold Atoms
Nguyen Duong Bo (Trung Tâm Vật Lý Lý Thuyết - Viện Vật Lý)

08:30 - 10:00 P.21 – Poster
Magneto-thermoelectric effects in doped semiconductor superlattice in the

presence of Laser radiation
Nguyen Quang Bau (Faculty of Physics, Hanoi University of Sciences, Vietnam National University)

08:30 - 10:00 P.22 – Poster
Elastic deformation of binary and ternary interstitial alloy with FCC structure at zero pressure: Dependence on temperature, concentration of substitution atoms and concentration of interstitial atoms
Nguyễn Đức Hiền (Sở GD & ĐT Gia Lai)

08:30 - 10:00 P.23 – Poster
A broadband laser-driven Kerr-like nonlinear coupler and entanglement
Doan Quoc Khoa (Quang Tri Teacher Training College)

08:30 - 10:00 P.24 – Poster
Anisotropic Magnetism of PdCo Ultrathin Film: Density Functional Theory Study
Do Son (Ho Chi Minh City University of Technology)

08:30 - 10:00 P.25 – Poster
Simple model for heating properties of protein-coated metallic nano-particles
Lương Thị Thêu (ĐHSP Hà Nội 2)

08:30 - 10:00 P.26 – Poster
Suppression of Cardiac Alternans by Chaotic Attractors
Le Duy Manh (Institute of Physics, VAST)

08:30 - 10:00 P.27 – Poster
Higher-order nonclassical properties of nonlinear charge pair cat states
Trương Minh Đức (Đại học Sư Phạm Huế)

08:30 - 10:00 P.28 – Poster
An application of q-deformed algebra to lattice vibrations
Nguyen Thi Ha Loan (Ha Noi Pedagogical University No. 2)

08:30 - 10:00 P.29 – Poster
Theoretical model for plasmonic properties of graphene-based nanostructures
Do Chi Nghia (Hanoi Pedagogical University No.2)

08:30 - 10:00 P.30 – Poster
The simplest 3-3-1 model
Le Tho Hue (Institute of Physics, VAST)

08:30 - 10:00 P.31 – Poster
Structure and dynamics of liquid Al2O3.2(SiO2) system as studied by Molecular Dynamics Simulation
Nguyen Van Yen (Hanoi University of Science and Technology)

08:30 - 10:00 P.32 – Poster
Evaluation the validity of the weak-field-approximation methods in consider-

ation of the ionization rate of atoms
Pham Nguyen Thanh Vinh (Ho Chi Minh University of Pedagogy)

08:30 - 10:00 P.33 – Poster
Optical cold atom trap with off-plane surface plasmon polaritons effect
Nguyen Thi Phuong Lan (Ha Noi Pedagogical University No. 2)

08:30 - 10:00 P.34 – Poster
Molecular Dynamics Simulation of Rutile – Anatase Heterojunction
Ca Nguyễn Anh Khoa (Đại học Cần Thơ)

08:30 - 10:00 P.35 – Poster
Precise calculations of average level spacing in even - even nuclei
Huong Thi Quynh Le (University of Khanh Hoa)

08:30 - 10:00 P.36 – Poster
Carbo principle of maximum quantum similarity and application in stock exchange markets
Chu Thuy Anh (Institute of Physics)

08:30 - 10:00 P.37 – Poster
Numerical solution of mean field theory for the three-component Ginzburg-Landau functional
Nguyen Van Hinh (Ha Noi University of industry)

08:30 - 10:00 P.38 – Poster
Energy spectrum inverse problem of q-deformed harmonic oscillator and entanglement of composite bosons
Sang Anh Nguyen (Hanoi Pedagogical University No.2)

08:30 - 10:00 P.39 – Poster
The electroweak theory based on SU(4)L X U(1)X gauge group
Duong Van Loi (Institute of Physics, VAST)

08:30 - 10:00 P.40 – Poster
A minimal 3-3-1 model for dark matter
Le Duc Thien (Hoang Van Thu High School for Gitted Students, Thinh Lang Precinct, Hoa Binh City, Hoa Binh Province, Viet Nam)

10:00 - 10:30 Coffee Break

Oral Session 4
Chair: Le Van Hoang

10:30 - 11:00 I.2 – Invited
Neutron noise simulation and application in diagnosis of fuel vibrations in a PWR
Tran Hoai Nam (Duy Tan University)

11:00 - 11:20 O.12 – Oral
Gauge Interactions from Compactification of Extra Dimensions

Dao Vong Duc (Institute of Physics, VAST)

11:20 - 11:40 O.13 – Oral

Toward a microscopic description of nucleon-nucleus scattering within the energy density functional approach

Nguyen Hoang Tung (Department of Nuclear Physics, University of Science, Ho Chi Minh City)

11:40 - 12:00 O.14 – Oral

On five-dimensional massive (bi)gravity

Do Q. Tuan (Vietnam National University, Hanoi)

12:00 - 14:00 Lunch Break

14:00 - 18:00 Excursion

18:00 - 20:30 Gala Dinner

Wednesday, 3 August 2016

Poster Session 2
Chair: Hoang Anh Tuan

08:30 - 10:00 P.41 – Poster

Sequence dependent aggregation of peptides and fibril growth

Nguyen Ba Hung (Vietnam Military Medical University)

08:30 - 10:00 P.42 – Poster

Network structure of SiO2 and MgSiO3 in amorphous and liquid States

Nguyễn Văn Hồng (Bộ môn Vật lý Tin học, Viện Vật lý Kỹ Thuật, ĐH Bách Khoa Hà Nội)

08:30 - 10:00 P.43 – Poster

Atomic structure of nanometer-sized amorphous TiO_2

Phan Thanh Hùng (Tra Vinh University)

08:30 - 10:00 P.44 – Poster

Growth of graphene by vapor deposition method and size effects on its structure.

Nguyen Hoang Giang (Comptutational Physics Lab, Institute of Technology, Vietnam National University - Ho Chi Minh City)

08:30 - 10:00 P.45 – Poster

Melting Boron Nitride Nanoribbons

Nguyen Hang (Ho Chi Minh City University of Technology)

08:30 - 10:00 P.46 – Poster

Uphill diffusion of vacancy in boron diffusion process in silicon

Vu Ba Dung (Hanoi University of Mining and Geology)

08:30 - 10:00 P.47 – Poster

Lepton flavor violating decay of neutral Higgs in seesaw models

Nguyễn Huy Thảo (Hanoi Pedagogical University 2)

08:30 - 10:00 P.48 – Poster

On the concentration dependence of metallic nano-particles in enhanced Forster resonance energy transfer

Nguyễn Minh Hoa (Hue University of Medicine and Pharmacy)

08:30 - 10:00 P.49 – Poster

The spatially anisotropic triangular lattice antiferromagnet: Popov-Fedotov method

Pham Thi Thanh Nga (Water Resources University)

08:30 - 10:00 P.50 – Poster

Thermodynamic property of interstitial alloy FeSi with vacancy and BCC structure: Dependence on temperature, concentration of interstitial atoms and concentration of equilibrium vacancies

Nguyễn Thị Hòa (University of Transport and Communications)

08:30 - 10:00 P.51 – Poster

Charge Creation from Extra Dimensions

Dao Vong Duc (Institute of Physics, VAST)

08:30 - 10:00 P.52 – Poster

Single-active-electron model potential for a polar molecule CO

Trần Lan Phương (Ho Chi Minh City University of Pedagogy)

08:30 - 10:00 P.53 – Poster

Phase diagram of hydrophobic thick ribbons

Trịnh Xuân Hoàng (Institute of Physics, VAST)

08:30 - 10:00 P.54 – Poster

Melting temperature and thermo-mechanical properties of iron in Debye model

Ho Khac Hieu (Duy Tan University)

08:30 - 10:00 P.55 – Poster

Influence of phonon confinement on the nonlinear optically detected electrophonon resonance linewidth in parabolic quantum wells

Tran Cong Phong (Vietnam Institute of Educational Sciences)

08:30 - 10:00 P.56 – Poster

Structural properties of amorphous 2D solid from the Liquid State with Square Potential

Nguyen To Nga (PetroVietnam University)

08:30 - 10:00 P.57 – Poster

Investigation of the nonsequential process of helium induced by two-color laser pulses

Truong Dang Hoai Thu (Ho Chi Minh University of Pedagogy)

08:30 - 10:00 P.58 – Poster

Study of crystallization mechanisms of Fe nanoparticle

Giap Thuy Trang (Thai Nguyen University of Education)

08:30 - 10:00 P.59 – Poster

Measurement of entanglement degree and controlled teleportation in the trio coherent states

Trương Minh Đức (Đại học Sư Phạm Huế)

08:30 - 10:00 P.60 – Poster

Negatively charged excitonin the atomic monolayer with the presence of a magnetic field

Nguyễn Phương Duy Anh (Thủ Dầu Một University)

08:30 - 10:00 P.61 – Poster

On the theory of three types of polaritons (phonon, exciton and surface plasmon polaritons)

Duong Thi Ha (Thai nguyen University of Education)

08:30 - 10:00 P.62 – Poster

Influence of an External Magnetic Field on the Acoustomagnetoelectric Field in a Cylindrical Quantum Wire with a Parabolic Potential

Nguyen Van Nghia (Thuy Loi University)

08:30 - 10:00 P.63 – Poster

Effects of phonons in the excitonic insulator in the 2D extended Falicov-Kimball model

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

08:30 - 10:00 P.64 – Poster

The orientation dependence of high-order harmonic generation and ionization probability of H2+ considering the nuclear vibration

Phan Thi Ngoc Loan (Ho Chi Minh City University of Pedagogy)

08:30 - 10:00 P.65 – Poster

Controllable electronics structure in Zigzag Bilayer Graphene nanoribbons

Nguyen Thi Kim Quyen (Can Tho University)

08:30 - 10:00 P.66 – Poster

A non–extensive thermodynamic theory of ecological systems

Le Van Xuan (Dong Xuan, Soc Son, Ha Noi, Viet Nam)

08:30 - 10:00 P.67 – Poster

Theoretical studies of energy band structure and density of state of Penta-Graphene

Pham Thanh Thuy (Can Tho University)

08:30 - 10:00 P.68 – Poster

Nuclear reactor calculations using MCNP6 code based on a CAD model

Nguyen Ba Vu Chinh (Danang University of Education)

08:30 - 10:00 P.69 – Poster

Simple model for dielectric constant of water at low frequencies

Tran Thi Nhan (Đại học Công Nghiệp Hà Nội)

08:30 - 10:00 P.70 – Poster

Metal-insulator transition in the standard three-component Falicov-Kimball model

Nguyen Duong Bo (Trung Tâm Vật Lý Lý Thuyết - Viện Vật Lý)

08:30 - 10:00 P.71 – Poster

On the existence of graphene-like liquid water structure

Le Tuan (Hanoi University of Science and Technology)

08:30 - 10:00 P.72 – Poster

Pressure-dependent structural heterogeneity in calcium silicate glass

Mai Thi Lan (Hanoi University of Sciences and Technology)

08:30 - 10:00 P.73 – Poster

Electron-phonon resonance linewidth in triangular quantum well via two-photon absorption process

Vinh Tuan Pham (Dong Thap University)

08:30 - 10:00 P.74 – Poster

Optical properties of Tamm states base on 1D Thue-Morse quasi-photonic crystals

Phung Duy Khuong (Institute of Physics)

08:30 - 10:00 P.75 – Poster

Influence of phonon confinement on the optically detected magneto-phonon resonance line-width in quantum wells

Nguyen Dinh Hien (Center for Theoretical and Computational Physics, Hue University's College of Education)

08:30 - 10:00 P.76 – Poster

Metal-insulator transitions in silicene with spin orbit-interaction

Nguyen Thi Huong (Thuy Loi University)

08:30 - 10:00 P.77 – Poster

Study on elastic deformation of AB substitution alloys with FCC structure at zero pressure

Nguyễn Đức Hiền (Sở GD & ĐT Gia Lai)

08:30 - 10:00 P.78 – Poster

Phenomenology of the 3-2-3-1 model

Duong Van Loi (Institute of Physics, VAST)

08:30 - 10:00 P.79 – Poster

Thermodynamic property of binary interstitial alloy with FCC structure: De-

pendence on temperature and concentration of interstitial atoms
Dinh Quang Vinh (Hanoi National University of Education)

10:00 - 10:30 Coffee Break

Oral Session 5
Chair: Dao Vong Duc

10:30 - 10:50 O.15 – Oral
Superintegrability of the nine-dimensional MICZ-Kepler problem
Phan Ngọc Hưng (HCMC University of Pedagogy)

10:50 - 11:10 O.16 – Oral
Octonionic representation of the nine-dimensional Micz-Kepler problem
Lê Đại Nam (Ton Duc Thang University)

11:10 - 11:30 O.17 – Oral
Lepton flavor violating decays of Standard-Model-like Higgs in 3-3-1 model with neutral lepton
Trương Trọng Thúc (NCS Viện Vật Lý)

11:30 - 11:50 O.18 – Oral
Lepton flavor violation processes in the charged lepton sector in minimal lepton flavor violation models
Dinh Nguyen Dinh (Institute of Physics, Hanoi)

12:00 - 14:00 Lunch Break

Oral Session 6
Chair: Pham Khac Hung

14:00 - 14:20 O.19 – Oral
Dynamical heterogeneity in supercooled liquid and glassy states of simple system
Nguyen Hoang Giang (Comptutational Physics Lab, Institute of Technology, Vietnam National University - Ho Chi Minh City)

14:20 - 14:40 O.20 – Oral
Thermoelectric and magnetic properties of gadolinium doped bismuth telluride: first-principles investigation
Tran Van Quang (Department of Physics, University of Transport and Communications and Institute of Research and Development, Duy Tan University)

14:40 - 15:00 O.21 – Oral
Theoretical prediction of ZnO hollow framework nanoporous structures
Vu Ngoc Tuoc (Hanoi University of Science and Technology)

15:00 - 15:20 O.22 – Oral
Pressure-induced structural transformation in SiO2 glass
Le Van Vinh (Department of Computational Physics, Hanoi University of Science and Technology, Vietnam)

15:30 - 16:00	Coffee Break
16:00 - 16:10	Closing
16:10 - 17:00	VTPS Meeting

Conference Abstracts

I.1 – Invited, NCTP-41

Ab initio study of Pd-skin/Pd3Fe(111) Electrocatalyst for oxygen reduction reaction

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Oxygen reduction reaction (ORR) is an important reaction occurring on the cathode electrocatalytic surface of proton exchange membrane fuel cells. Developing new electrocatalysts by alloying inexpensive metals other than the well-known but expensive Pt is one of the most feasible and economical schemes to improve the performance of the fuel cells to a practical level. Electrocatalysts of Pd-skin/Pd3Fe(111) alloy have emerged as one of the most promising candidates. However, no detailed researches are available for the ORR activity and the stability of this alloy in the ORR environment. Therefore, we employed the density functional theory calculations to study the Pd-skin/Pd3Fe(111) alloy to clarify the following subjects: (1) the ORR activity, (2) the stability of Pd-skin/Pd3Fe(111) alloy, and (3) effects of electrode potential on the formation of the ORR intermediates. The results will be useful for a rational design of better electrocatalytic cathodes for proton exchange membrane fuel cells.

Acknowledgement This research is funded by the Ho Chi Minh City Department of Science and Technology.

Presenter: Do Son

I.2 – Invited, NCTP-41

Neutron noise simulation and application in diagnosis of fuel vibrations in a PWR

Tran Hoai Nam

Duy Tan University

Neutron noise is the fluctuation of neutron flux in the reactor core due to in-core fluctuations. The fluctuations is due to physical and technological processes, such as fluctuations in temperature, pressure, density, and displacement of reactor components. These processes lead to the changes of macroscopic cross sections, and therefore, affecting neutron flux. The neutron noise

could be measured by detectors located inside and/or outside of the core. Neutron noise analysis has been early considered as a powerful technique in reactor diagnostics and core monitoring. Online diagnostics for monitoring the operating status of light water reactors (LWRs) based on analyzing the detector signals of neutron noise were deployed widely in various countries. Numerical simulation based on solving the neutron noise equation in diffusion theory in a frequency domain remains a challenge to reproduce and interpret the measured data. In this report, we present the recent development of numerical simulations of the neutron noise in power reactors. Application in investigating the characteristics of the neutron noise induced by the in-core fuel assembly vibrations in PWRs will also be presented.

Presenter: Tran Hoai Nam

O.1 – Oral, NCTP-41

Atom-atom and atom-body dispersion potential in a cylindrical system

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Atom-atom and atom-body dispersion interaction is influenced by the presence of macroscopic bodies nearby. By suitably manipulating the macroscopic bodies, one can efficiently control the dispersion interaction, leading to potential applications in fields as diverge as biologically based electronics and methane gas extraction from shale-gas systems. Here we consider the atom-atom and atom-body dispersion interaction in the presence of a cylindrical waveguide, focusing on the effects of the atomic dipole orientations and the finite length of the waveguides. In particular, in the case of atoms having radial dipole moments and being located outside a waveguide, the interatomic dispersion interaction is found to be strongly enhanced as compared with that in free space. Results for a perfectly reflecting wall and walls made of a conductor (gold) and a dielectric (undoped silicon) are compared. It is shown that though the perfectly reflecting waveguide model can predict qualitatively correctly the main features of the interatomic dispersion interaction, taking into account realistic permittivities is important because the difference can amount to a few orders of magnitudes.

Presenter: Nguyen Dung Chinh

O.2 – Oral, NCTP-41

Higher order non-classicalities in the Kerr-like coupler systems

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In this paper, we show the existence of various types of non-classical effects in the model of the nonlinear Kerr-coupler containing two quantum nonlinear oscilators mutually coupled by continuous nonlinear interaction, such as squeezing, anti-bunching, intermodal entanglement and their higher order counterparts. By using unitary evolution operator formalism and the common inequalities expressed in term of various moments defined by products of creation and annihilation operators, we find numerically the "exact" solutions of these factors for both cases non-dissipative and dissipation regimes. We show and discuss the parameters considered can be indicators of generation such nonclassical effects and hence, quantumness of the system.

Presenter: Nguyen Thi Dung

O.3 – Oral, NCTP-41

A study of supersolid phase in square lattice Bose Hubbard model at finite temperature using quantum Monte Carlo simulation

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The behavior of supersolid phase at finite temperature has been investigated using quantum Monte Carlo - Worm Algorithm. The nearest and next nearest neighbor interaction Bose Hubbard model is chosen as a minimum model of supersolid phase in square lattice. The appearance of supersolid phase at zero temperature driven by interaction at zero temperature will be represented by the two order parameters which are superfluid density and static structure factor. QMC is able to access these different order parameters which are responsible for the different phases such as superfluid, supersolid as well as the crystal phases. It is also doable to investigate the system at finite temperature, hence the phase transition. As shown in this work, these supersolid order paramters also survive at finite temperature. The rich phase diagram has been achieved and the critical exponents falls into XY-universality class will be examined. The Kosterlitz - Thouless phase transition will also be discussed. The work aims to explain the possible experiment in optical lattice and helium absorbed on top of graphite.

Presenter: Dang Dinh Long

O.4 – Oral, NCTP-41

Two-component fermions in optical lattice with spatially alternating interactions

Hoang Anh Tuan (1), Nguyen Thi Hai Yen (1), Tran Thi Thu Trang (2) and Le Duc Anh (3)

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We investigate two-component mass-imbalanced fermions in optical lattice with spatially modulated interactions by using the two-site dynamical mean field theory. At half-filling and zero temperature, the phase diagram of the system is analytically obtained, where a metallic region is reduced with increasing the mass imbalance. Ground state properties of the fermionic system are discussed from behaviors of both the quasi-particle weight at the Fermi level for each component and the double occupancy for each sublattice as functions of the local interaction strengths for various values of the mass imbalance.

Presenter: Nguyen Thi Hai Yen

O.5 – Oral, NCTP-41

Strutural organization and network structure of liquid zircon under compression

Tran Thuy Duong, Nguyen Van Hong

Hanoi University of Science and Technology

Strutural organization and network structure of liquid zircon (ZrSiO4) under a wide pressure

range are investigated by molecular dynamics simulation and visualization. The short range order (SRO) and intermediate range order (IRO) characteristics are analyzed via topology statistics of basic structural units TOn and likages OTm (T=Zr, Si). Investigation results of network structure and size distribution of Si-O and Zr-O subnets show that the structure of zircon decomposes into ZrO2- and SiO2-rich regions. The micro-phase separation and structural and compositional heterogeneities of ZrSiO4 are also discussed in this work.

Presenter: Tran Thuy Duong

O.6 – Oral, NCTP-41

First-Principles Study on Electronic Structures and Oxygen Vacancy Formation in Strained LaNiO3 Structures

Huy Duy Nguyen, Duy Ba Pham, and Bach Thanh Cong

VNU University of Science

The LaNiO3 is a rare perovskite oxide that exhibits paramagnetic metallic behavior, and is frequently utilized in the cathode materials for solid oxide fuel cells (SOFCs) [1]. The usage of LaNiO3 in SOFCs stems from the ability to catalyze the oxygen reduction reaction (ORR), as well as the high-temperature stability and acceptable thermal expansion properties. In the ORR process, oxygen vacancies are important as the vacancies can strongly couple to the oxygen dissociation, transport, and incorporation. Previous theoretical work based on first-principles calculations have predicted that bulk LaNiO3 has a much stronger preference for oxygen vacancy formation compared to SrTiO3 [2]. However, as LaNiO3 is always deposited on a substrate, the effect of interfacial strain on the formation of oxygen vacancy is important, and to the best of our knowledge, number of studies on such matter is limited. In this paper, we study the effects of interfacial strain on the electronic structures and the oxygen vacancy formation in LaNiO3 structures. The first-principles calculations are carried out within the framework of density functional theory using a plane wave basis set, as implemented in the quantum espresso software package. The electron-ion interaction is described using Vanderbilt ultrasoft pseudopotentials, and the exchange-correlation interaction is treated by the local density approximation. The interfacial strain is simulated by changing the lattice parameters in the *xy* plane and allow the structure to relax in the z direction. We investigate the 2x2x2 LaNiO3 supercell and find that the optimized bulk structure exhibits clear local distortions of NiO6 octahedrals, i.e., the octahedrals are titled in correlation to each other. The tilting is suppressed (enhanced) in the case of compressive (tensile) strains. This octahedral tilting results in the reduction of the hybridization between O 2p and Ni 3d states. By plotting the local densities of states, we confirm that O pz- and Ni e2g-derived states become more localized as the Ni-O-Ni angle along the z direction decreases. The oxygen vacancy is investigated by removing one oxygen atom in the LaO or NiO2 layer, and the dependence of oxygen vacancy formation energy (EVO) on the in-plane strain for a missing oxygen in LaO and NiO2 layer, relative to the EVO in the unstrained structure, is studied. It is found that EVO for a missing oxygen in the NiO2 layer decreases by applying both compressive or tensile strains. On the contrary, the EVO for a missing oxygen in the LaO-layer increases (decreases) as the compressive (tensile) strain increases. This behavior is attributed to the reduction in the hybridization between O pz and Ni e2g states in the case of tensile strain leading to the decrease in EVO. Our results indicate that interfacial strains can be utilized to modify the oxygen vacancy concentration in the bulk LaNiO3.

References [1] S. B. Adler, Chem. Rev. (Washington, D.C.) 104, 4791 (2004). [2] A. Malashevich and S. Ismail-Beigi, Phys. Rev. B 92, 144102 (2015).

Presenter: Nguyen Duy Huy

O.7 – Oral, NCTP-41

Grand-canonical Monte-Carlo simulation of salt mixtures and an application to study osmotic pressure of DNA bundle

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A Grand-canonical Monte-Carlo simulation method extended to simulate a mixture of salts using primitive ion models is presented. The fugacities for different salts or salts mixtures at different concentrations are reported. The results are applied to study numerically the osmotic pressure of DNA hexagonal bundle in equilibrium with a bulk solution of salt mixture of monovalent and divalent counterions. Experimentally, it is know, that multivalent counterions have strong effect on the DNA condensation phenomenon. While tri- and tetra-valent counterions are shown to easily condense free DNA molecules in solution into toroidal bundles. Some divalent counterions like Mg^{+2} are not able to condense free DNA molecules in solution, while some like Mn^{+2} can condense them into disorder bundles. In restricted environment such as in two dimensional system or inside viral capsid, Mg^{+2} can have strong effect and able to condense them, but the condensation varies qualitatively with different system, different coions. Our simulations show that, varying the divalent salt concentration and ion sizes has considerable effect on the osmotic pressure, in qualitative agreement with experimental results. This paper is to delicate to Dr. Peter Brommer – a former physicist of the University of Amsterdam.

Presenter: Nguyen Viet Duc

O.8 – Oral, NCTP-41

Modulation of bandgap in armchair bilayer graphene ribbons: a comparison between vertical and transverse fields

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The electronic bandgap is an intrinsic property of semiconductors and insulators that largely determines their electrical and optical properties. As such, it has a central role in modern device physics and technology, and governs the operation of semiconductor devices such as p–n junctions, transistors, photodiodes and lasers. A tunable bandgap would be highly desirable because it would allow greater flexibility in design and optimization of such devices, in particular, if it could be tuned by applying variable external electric fields. Here we theoretically investigate the effects of a transverse electric field (generated by side gates), and a vertical electric field (generated by top/back gates) on energy bands, and transport properties of armchair bilayer graphene ribbons (Bernal stacking). Using atomistic Tight Binding calculations and Green's function formalism, we demonstrate that bandgap is opened when either field is applied and

even enlarged under simultaneous influences of the two fields. The results also illustrated that armchair bilayer graphene ribbons always exhibits three classes such as 3p, 3p+1, 3p+2 in which the gap decreases as the ribbon width increases and eventually approaches metallicity like an infinite Graphene. Interestingly, although vertical electric fields are widely used to control band gap in bilayer graphene, here we also show that vertical fields exhibit more positive effects in terms of modulating a larger band gap and these results are totally different from the ones we obtained for zigzag bilayer graphene ribbons. These results may motivate new device designs made of bilayer graphene ribbons using electric gates. Combined with the remarkable electrical transport properties of such systems, this electrostatic bandgap control suggests novel nano-electronic and nanophotonic device applications based on graphene. This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2015.98

Presenter: Vu Thanh Tra

O.9 – Oral, NCTP-41

Magnetic and topological transitions in an insulator with doped magnetic impurities

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Magnetic and topological transitions in an insulator doped with magnetic impurities is studied based on an interplay between the spin-orbit coupling of electrons and the spin exchange of these electrons with magnetic impurity moments. The model is constructed based on the Kane-Mele model in the presence of magnetic impurities. The magnetic and topological transitions are detected by monitoring the topological invariant and the spontaneous magnetization, which are self consistently determined within the dynamical mean-field theory. We find different magnetic topological phase transitions, depending on the electron filling. At half filling an antiferromagnetic topological insulator, which exhibits the quantum spin Hall effect, exists in the phase region between the paramagnetic topological insulator and the trivially topological antiferromagnetic insulator. At quarter and three quarters fillings, a ferromagnetic topological insulator, which exhibits the quantum anomalous Hall effect, occurs in the strong spin-exchange regime.

Presenter: Nguyen Hong Son

O.10 – Oral, NCTP-41

The main scattering mechanisms in Single-side modulation doped square quantum wells

Trần Thị Hải, Nguyễn Mạnh An, Nguyễn Thị Dung

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We present a theory of the transport of electrons confined in the conduction band of a single-side modulation doped square quantum wells. Beside the well-known the scattering mechanisms

such as surface roughness and Alloy disorder, the theory induces acoustic phonon due to the deformation potential and acoustic phonon due to the piezoelectric coupling. The result we prove that acoustic phonon scattering has revealed very large mobility values. We have also consider acoustic-phonon partial mobility dependece on temperature for single-side modulation doped square quantum wells.

Presenter: Trần Thị Hải

O.11 – Oral, NCTP-41

High-order harmonic generation by using single-active electron model potential

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The study of high-order harmonic generation (HHG) from molecules is a subject of much current interest of science. To explain the features of the HHG, some methods of ab initial calculations are introduced, such asthe time-dependent density functional theory (TDDFT), the time-dependent Hartree-Fock method (TDHF). In our work, we develop an alternative method to calculate HHG spectra for molecules within the single-active-electron (SAE) approximation. Firstly,the single-active-electron potential of a molecule CO2is constructed with using the initial wave function obtained from GAUSSIAN 03. Secondly, the time-dependent Schrodinger equation of the molecule interacted with the ultrashort laser pulses is solved numerically by the split-operator method. Then, the HHG spectra for different alignment angles are calculated and compared to those of other numerical calculations. Using the obtained data of HHG, we analyze the possibility of extracting the structural information of CO2 by applyingthe electron interference effect.

Presenter: Le Thi Cam Tu

O.12 – Oral, NCTP-41

Gauge Interactions from Compactification of Extra Dimensions

Dao Vong Duc

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Within the framework of the mechanism proposed in our previons works for mass and charge creation (DV Duc and NM Giao, J. Mod. Phys. 4, 991, 2013, DV Duc et al. J, Phys. Sci. Appl. 4, 60, 2014, DV Duc and NM Giao, Int. J, Theor. Phys. 54, 1071, 2015, DV Duc and NM Giao, Int. J, Theor. Phys. 55, 959, 2016), we consider the case of non-abelian gauge interactions. The expressions for traditional interaction Lagrangians are obtained, based on some specific assumptions related to the geometrie topology of extradimensions.

Presenter: Dao Vong Duc

O.13 – Oral, NCTP-41

Toward a microscopic description of nucleon-nucleus scattering within the energy density functional approach

N. Hoang Tung (1, 2, 3), N. Nhu Le (4), Meng-Hock Koh (5), H. N. Tran (1, 2), Vinh N. T. Pham (6), T. V. Nhan Hao (7, 8)

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A fully self-consistent framework of the particle-vibration coupling [1] is applied to generate the microscopic nucleon-nucleus optical potential. The effective interaction Skyrme has been consistently used to describe the mean-field, the excited states of the target, and the particle state collective couplings. For the first time, microscopic description of low energy nucleon-nucleus scattering off a series of double-closed shell nuclei 16O, 40Ca, 48Ca, 208Pb is completely carried out without any adjustable parameter. The sensitivity and consistence of choosing interactions to the calculations of nuclear reaction observables are analyzed. Angular distributions of the evaluated data are successfully reproduced.

[1] T. V. Nhan Hao, B. Minh Loc, and N. Hoang Phuc, Phys. Rev. C 92, 014605 (2015).

Presenter: Nguyen Hoang Tung

O.14 – Oral, NCTP-41

On five-dimensional massive (bi)gravity

Tuan Q. Do

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Main results of our recent investigations on five-dimensional scenarios of massive (bi)gravity will be presented in this talk. In particular, we will show how to construct higher dimensional massive graviton terms from the characteristic equation of square matrix, which is a consequence of the Cayley-Hamilton theorem. Then, we will show whether massive graviton terms of five-dimensional massive (bi)gravity behave as effective cosmological constants for a number of physical metrics compatible with fiducial ones such as the Friedmann-Lemaitre-Robertson-Walker, Bianchi type I, and Schwarzschild-Tangherlini metrics. Finally, we will show the corresponding cosmological solutions for the five-dimensional massive (bi)gravity.

Presenter: Do Q. Tuan

O.15 – Oral, NCTP-41

Superintegrability of the nine-dimensional MICZ-Kepler problem

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The nine-dimensional MICZ-Kepler system with the SO(8) monopole potential has been regarded to have SO(10) symmetry recently. Based on this symmetry, we built a set of seventeen second order invariant operators including the Hamiltonian of the system that satisfies the superintegrable condition. Furthermore, we also show that the algebra generated by these sec-

ond order symmetries is closed under commutation relation. This means the nine-dimensional MICZ-Kepler problem is maximally superintegrable.

Presenter: Phan Ngọc Hưng

O.16 – Oral, NCTP-41

Octonionic representation of the nine-dimensional Micz-Kepler problem

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In previous works, it was proved that the connection between the 2^{h+1}-dimensional isotropic harmonic oscillator problem and the $(2h+1)$-dimensional MICZ-Kepler problem via the h-th Hurwitz transformation can be established only for. On other hand, each h-th Hurwitz transformations is directly related to the h-th normed division algebra. In present report, we consider the last case where the generalized Hurwitz transformation can be represented by the last normed division algebra, octonion. By using the above-mentioned connection, we can describe the nine dimensional MICZ-Kepler problem in the octonionic representation. Some discussions about the SO(8) monopoles are carried out in the light of the connection between the 16-dimensional isotropic harmonic oscillator and the 9-dimensional MICZ-Kepler problems by the normed division algebras.

Presenter: Lê Đại Nam

O.17 – Oral, NCTP-41

Lepton flavor violating decays of Standard-Model-like Higgs in 3-3-1 model with neutral lepton

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The one loop contribution to the lepton flavor violating decay $h^0 \to \mu\tau$ of the SM-like neutral Higgs (LFVHD) in the 3-3-1 model with neutral lepton (3-3-1LHN) is calculated using the unitary gauge. We will represent the particle spectrum and couplings relating with LFVHD decay process. Contributions of particular diagrams and divergent cancelation are shown. Based on numerical investigation, we show that the branching ratio of the LFVHD strongly depends on the Yukawa couplings between exotic leptons and $SU(3)_L$ Higgs triplets. **This ratio can reach** 10^{-5} **providing large Yukawa couplings and constructive correlations of the** $SU(3)_L$ **scale** (v_3) **and the charged Higgs masses**. The branching ratio decreases rapidly with the small Yukawa couplings and large v_3.

Presenter: Trương Trọng Thúc

O.18 – Oral, NCTP-41

Lepton flavor violation processes in the charged lepton sector in minimal lepton flavor violation models

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In this report, we discuss lepton flavor violation in some typical scenarios of minimal lepton flavor violation (MLFV). We introduce briefly the MLFV models in the three following scenarios: i, the Standard Model (SM) field content basing on lepton flavor group $G_{LF} = SU(3)_L \times SU(3)_{E_R}$; the see-saw type I field contents with three heavy right-handed neutrinos, and the lepton flavor group $G_{ELF} = SU(3)_L \times SU(3)_{E_R} \times SU(3)_{\nu_R} = G_{LF} \times SU(3)_{\nu_R}$, in cases: ii, $SU(3)_{\nu_R} \to O(3)_{\nu_R} \times \mathrm{CP}$; and iii, $SU(3)_L \times SU(3)_{\nu_R} \to SU(3)_{L+\nu_R}$. The branching ratios of LFV processes, such as $\ell \to \ell' + \gamma$, $\ell \to 3\ell'$, and the conversion ratio of $\mu - e$ conversion, will be introduced and analyzed using the current neutrino oscillation experimental data.

Presenter: Dinh Nguyen Dinh

O.19 – Oral, NCTP-41

Dynamical heterogeneity in supercooled liquid and glassy states of simple system

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We present molecular dynamics (MD) simulations of dynamical heterogeneity in 3D simple monatomic supercooled liquid and glassy states obtained by cooling from liquid to glassy state. Models contain 8000 particles interacted via Lennard-Jones-Gauss potential. Evolution of structure and various thermodynamic properties upon cooling from liquid to glassy state is analyzed in details via radial distribution function (RDF), temperature dependence of total energy, mass density, time – temperature dependence of mean - squared displacement (MSD), temperature dependence of fraction of atoms with diffferent mobilities, size of the largest cluster and mean cluster size of atoms, fraction of solidlike atoms, 3D visualization of atomic configurations. Via intensive MD simulation of glass formation in 3D simple supercooled liquids we find that atoms with the same or close mobilities have a tendency to aggregate into clusters. With decreasing temperature, fraction of these atoms passes over a maximum and then it decreases downto zero. In contrast, fraction of solidlike atoms (i.e. with the slowest mobility) increases monotonously with a sudden increase in the vicinity of glass transition reaching almost 100

Presenter: Nguyen Hoang Giang

O.20 – Oral, NCTP-41

Thermoelectric and magnetic properties of gadolinium doped bismuth telluride: first-principles investigation

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Bismuth telluride with doped magnetic elements have been great of interest in the years due to its potential application as thermoelectrical materials and the unique electronic structures related to the topological insulator. Especially, rare earth doping reveals many exotic magnetic property change in host materials. In this work, within the density functional theory, we perform first-principles electronic structure calculation by employing the all-electron full-potential

linearized augmented planewave (FLAPW) method [1] to examine magnetic properties and thermoelectric properties of Gd doped bismuth telluride. Results show that Gd substituted alloy is ferromagnetic with the magnetic moment of $7\mu B$ which purely comes from f-states of Gd atoms. The strong correlation and spin-orbital coupling effects are crucial to describe the electronic structure of the alloy. Interaction between the valence electrons produces semimetallic Gd-Bi2Te3, which enhances the electrical conductivity, but decrease the Seebeck coefficient on the other hand. To substantiate this point, we calculate the Seebeck coefficient, the electrical conductivity, and the thermoelectric power factor by utilizing the FLAPW wave-functions and the solution of Boltzmann transport equation in a constant relaxation-time approximation.

[1] E. Wimmer, H. Krakauer, M. Weinert, and A. J. Freeman, Phys. Rev. B 24, 864 (1981).

Presenter: Tran Van Quang

O.21 – Oral, NCTP-41

Theoretical prediction of ZnO hollow framework nanoporous structures

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Along with wurtzite and zinblende, zinc oxide (ZnO) has been found in a large number of polymorphs with substantially different properties, and hence, applications. Therefore, predicting and synthesizing new classes of ZnO polymorphs is of great significance and has been gaining considerable interest. Herein, we perform a density functional theory based study, predicting several new series of ZnO flexible hollow structures using the bottom-up design approach. For the structural phase stability, our calculations show that these hollow structures could survive in periodic systems without structural collapse, which leads to nanoporous low-density phases of ZnO. We found that the bulk modulus have saturated at certain hollow's wall thickness regarding to hollow-to-bulk density ratio. Consequently, for the purpose of low-density geometry engineering, the optimal value for strength-to-density figure of merit should reach a certain critical thickness. Their room temperature stability is discussed by means of the free energy computed within the lattice-dynamics approach. Our calculations also indicate that all the reported nanoporous structures, if synthesized, would preserve the valuable properties of the ZnO materials, e.g. wide bandgap semiconducting, piezoelectric and optically transparent, while, at the same time, would possess novel properties as of band flattening and gap engineering possibility. The electronic band structures of the ZnO hollow structures are finally examined in details.

Presenter: Vu Ngoc Tuoc

O.22 – Oral, NCTP-41

Pressure-induced structural transformation in SiO2 glass

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Molecular dynamics (MD) simulations of SiO2 glass been carried out to investigate the pressure-induced structural transformation. We found that not only the faction of units SiOx (x=4, 5,

6) but also the density of each SiOx type change upon compression. The density of sample can be expressed through the fraction and one of units SiOx. With increasing pressure, O atoms are more ordered than Si atoms and to form fcc and hcp clusters. The same units SiOx link together to form atomic clusters (AC) of type AC4, AC5 and AC6.

Presenter: Le Van Vinh

P.1 – Poster, NCTP-41

Hydrogen storage in MIL-88: Computational study

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Metal organic frameworks (MOFs) are considered as the most potential candidate for hydrogen adsorption. MIL-88 series is very stable toward humidity and hence suitable for hydrogen adsorption. However, no researches are available to evaluate the hydrogen storage capability of MIL-88. Here, we use the density functional theory calculations and Monte Carlo simulations to study adsorption isotherms, isosteric heats of adsorption, and Henry coefficient. Through the analysis of these quantities, we gauge the performance of MIL-88 for hydrogen storage in comparison with other MOFs. Acknowledgement This research is funded by Ho Chi Minh City University of Technology under grant number SVCQ-2015-KHUD-31

Presenter: O My Na

P.2 – Poster, NCTP-41

Phonon-assisted cyclotron resonance in MoS2 on polar substrates via two photon absorption process

Huynh Vinh Phuc (1), Luong Van Tung (1), Le Dinh (2), Tran Cong Phong (2,3)

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In this work, we study the influence of surface optical (SO) phonons on the phonon-assisted cyclotron resonance (PACR) effect in a monolayer MoS2 on different polar substrates via both one and two-photon absorption processes. The two-photon absorption process gives a significant contribution to magneto-optical absorption coefficient (MOAC) compared to one photon process. The shifts of the absorption peaks are larger for polar substrates than those in MoS2 on nonpolar substrates, where only the intrinsic optical phonons of MoS2 with higher energy contribute. Effects of temperature, MoS2-substrate thickness, and magnetic field on MOAC and full width at half maximum (FWHM) are discussed.

Presenter: Huỳnh Vĩnh Phúc

P.3 – Poster, NCTP-41

Metal-insulator phase diagram for the fully diagonal disordered Hubbard model at half-filling

Hoang Anh Tuan (1) and Nguyen Thi Hai Yen (1)

Institute of Physics, VAST

The electronic properties of strongly correlated systems with binary type of disorder are investigated using the coherent potential approximation. For half-filled systems, two transitions from a band insulator via a metallic state to a Mott insulator are found with increasing the local Coulomb repulsion of only one of the constituents. Our phase diagram is compared with those obtained by the dynamical mean field theory.

Presenter: Hoang Anh-Tuan

P.4 – Poster, NCTP-41

Protection of a non-Fermi liquid by spin-orbit interaction

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

(1) Institute of Physics, Vietnam Academy of Science and Technology (2) Abdus Salam International Centre for Theoretical Physics

We show that a thermo-electric transport through a Quantum Dot - single-mode Quantum Point Contact nano-device demonstrating pronounced fingerprints of Non-Fermi Liquid (NFL) behavior in the absence of external magnetic field is protected from magnetic field NFL destruction by strong spin-orbit interaction (SOI). The mechanism of protection is associated with appearance of additional scattering processes due to lack of spin conservation in the presence of both SOI and small Zeemann field. The interplay between in-plane magnetic field $\vec{B}$ and SOI is controlled by the angle between $\vec{B}$ and $\vec{B}_{SOI}$. We predict strong dependence of the thermo-electric coefficients on the orientation of the magnetic field and discuss a window of parameters for experimental observation of NFL effects.

Presenter: Nguyen Thi Kim Thanh

P.5 – Poster, NCTP-41

Spontaneous decay rate of a two-level atom in the presence of a multilayered-cylindrical waveguide

Tran Minh Hien (1) and Ho Trung Dung (2,3)

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We consider the spontaneous decay rate of a two-level excited atom positioned in a multilayered-cylindrical waveguide. We focus on the direction of dipole moment parallel to the cylinder axis. Three types of configuration are studied including a three-layer Drude-Lorentz type, a four-layer Lorentz-bandgap type, and a Bragg-distributed mirror type. It is shown that, if the atom is located inside of the waveguide, in the bandgap between the transverse and the longditudinal frequency of the medium filling the wall of the resonator, the atom can be trapped in the excited state. Beside, the decay rate experiences most pronounced modifications in the bandgap of the wall of the mirror. The level Lamb shift is also considered in detail.

Presenter: Trần Minh Hiến

P.6 – Poster, NCTP-41

Electronic properties of monolayer molybdenum disulphide under strain: An ab-initio calculations

Nguyen Van Chuong (1), Le Cong Nhan (2), Nguyen Van Hieu (3), Nguyen Ngoc Hieu (4)

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We investigated the structural properties and electronic states of monolayer MoS_2 under uniaxial/biaxial strain using density functional theory. At the equilibrium state, MoS_2 has a direct band gap of 1.72 eV opening at the K-point. The indirect–direct band gap transition has been found in MoS_2 monolayer when the strain was introduced. MoS_2 becomes a semiconductor with an indirect band gap when the unixial strain $\varepsilon_x \geq 1\%$ or the biaxial strain $\varepsilon_{xy} \geq 1\%$. Under biaxial strain, a metal–semiconductor transition occurs at 18% of elongation.

Presenter: Nguyen Ngoc Hieu

P.7 – Poster, NCTP-41

Effects of external electric fields on transmission and Seebeck coefficients in Bilayer Graphene nanoribbons

Vu Thanh Tra (1), Nguyen Thi Kim Hue (2), Tran Van Nhan (2)

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Graphene has shown great applications as the host material for next-generation electronic devices. Previous research demonstrated monolayer Graphene has metallicity, however, Bilayer Graphene exhibits semi-metal characteristics. We have successfully controlled bandgap of AB stacking in Bilayer Graphene by using the external electric fields. Based on the modulation of these electronic structures, calculated by Tight-Binding methods, with field strength is reflected in their electrical properties and Seebeck coefficients. Using Green's function formalism, we continue to examine the transmission and Seebeck coefficients. Interestingly, we recognize that the transmission and Seebeck coeffients strongly depend on transverse electric fields rather than vertical ones. More importantly, we discriminate the electronic and thermal properties between Armchair and Zigzag Bilayer Graphene nanoribbons. These results may attract new engineering device designs made of Bilayer Graphene nanoribbons. This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2015.98

Presenter: Nguyen Thi Kim Hue

P.8 – Poster, NCTP-41

Some applications using the connection between q-deformed harmonic oscillator and two types of symmetric and asymmetric harmonic potentials

Ngo Gia Vinh (1), Man Van Ngu (2), Nguyen Thi Dung (3), Nguyen Tri Lan (4), Luu Thi Kim Thanh (5), Nguyen Ai Viet (4)

(1) Bac Ninh Department of Education and Training; (2) Hung Yen Industrial Colleage; (3) Bacninh teacher training College; (4) Institute of Physics, 10 Dao Tan, Ba Dinh, Hanoi; (5) Hanoi Pedagogical University No.2

In our previous article, the connections between q-deformed harmonic oscillator and the two types of asymmetric (Morse-like) and symmetric (inverse square cosine form) potentials and are investigated. Using these relations in inverse way to investigate the properties of q-deformed harmonic oscillators is proposed. In this work we explore possibility of using this approach to study some real physical problems, such as diatomic molecules, phonon, etc.

Presenter: Ngô Gia Vịnh

P.9 – Poster, NCTP-41

Derivation of the general formula to describe the Stark shifted energy for Hydrogen atom under the influence of static electric field

Tran Duong Anh Tai (1), Ho Hoang Huy (1), Pham Nguyen Thanh Vinh (1)

(1) Ho Chi Minh University of Pedagogy

In this study, we propose a rigorous procedure to derive the analytical formula that is able to describe the Stark shifted energy for arbitrary state of Hydrogen atom when it is exposed to a uniform electric field. The general formula is constructed up to second order of perturbation theory in the parabolic coordinates which are convenient to separate the variables. The applicability of the analytical formula is validated by comparison with the exactly numerical calculation. The result indicates that the formula can be applied up to 0.2 a.u. in field strength for the ground state of hydrogen atom.

Presenter: Pham Nguyen Thanh Vinh

P.10 – Poster, NCTP-41

Investigation of thermodynamic and mechanical properties of AlxIn1-xP alloys by Statistical Moment Method

Vu Thi Thanh Ha (1), Vu Van Hung (2), Pham Thi Minh Hanh (3) and Ho Khac Hieu (4)

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In this work, the thermodynamic and mechanical properties of III-V zinc-blende AlP, InP semiconductors and their alloy have been studied in detail from statistical moment method taking into account the anharmonicity effects of the lattice vibrations. The nearest neighbor distance, thermal expansion coefficient, bulk moduli, specific heats at the constant volume and constant pressure of the zincblende AlP, InP and AlxIn1–xP alloy are calculated as a function of the temperature. The statistical moment method calculations are performed by using the many-body Stilinger-Weber potential. The concentration dependences of the thermodynamic quantities of zincblende AlxIn1–xP crystals have also been discussed and compared with those of the experimental results.

Presenter: Ho Khac Hieu

P.11 – Poster, NCTP-41

Invariance of probability density functions and transition between Gaussian and Boltzmann forms of envelope functions problem in the similarity between q-deform harmonic oscillator and Cooper pair

Man Van Ngu (1), Ngo Gia Vinh (2), Tran Ngoc Tu (3), Nguyen Tri Lan (4), Luu Thi Kim Thanh (5), Nguyen Ai Viet (4)

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The similarity of a Cooper pair and q-deform harmonic oscillator was discussed in our previous work, where have shown that the main different is the forms of their envelope functions. The envelope function of a Cooper pair has the Boltzmann-like form, while the envelope function of q-deform harmonic oscillator has the Gaussian-like form. In this work we analyze the invariance of probability density functions by a general transformation. We show that translation invariance corresponds to the Boltzmann-like form, and spherical invariance corresponds to the Gaussian-like form of probability density functions. Following the famous Einstein's idea about the connection between interaction and geometry of vacuum, we propose a possible transformation envelope function of a q-deform harmonic oscillator from Gaussian-like to Boltzmann-like forms, which correspond to the changing of an effective vacuum symmetrical behavior of a Cooper pair from its normal to superconducting states near the phase transition critical temperature.

Presenter: Mẫn Văn Ngữ

P.12 – Poster, NCTP-41

Quality of joint remote state preparation subjected to noises

Nguyen Van Hop (1), Cao Thi Bich (2) and Nguyen Ba An (2)

(1) Department of Physics, Hanoi National University of Education; (2) Center for Theoretical Physics, Institute of Physics, VAST

We investigate joint remote state preparation in the presence of noises caused by surrounding environments. We consider all possible noisy scenarios experienced by some or all the qubits of the shared quantum channel. The results cannot be described in a general manner so case-by-case analyses must be carried out. In particular, we show that quality of the prepared state is better when the qubits are subjected to optimal combinations of different types of noises than when they undergo the same noise type. Furthermore, we indicate that under certain scenarios less entanglement or more noise may make the preparation process more efficient.

Presenter: Nguyen Van Hop

P.13 – Poster, NCTP-41

Thermodynamic properties of thin films described by the transverse Ising model

Nguyen Tu Niem, Bach Huong Giang, Bach Thanh Cong

Computational Materials Science Laboratory, Faculty of Physics, VNU University of Science

Functional integral method is employed to calculate thermodynamic properties of thin ferroic (ferromagnetic or ferroelectric) films within the framework of a transverse Ising model. The conventional mean field approximation for free energy and for equation of states is carried out with higher-order correction by using Gaussian approximations. We also analyze the dependence of fluctuations of the order parameter on temperature and on the thickness of thin films.

Presenter: Nguyễn Từ Niệm

P.14 – Poster, NCTP-41

Cooling rate effects on formation of 2D solid with square lattice structure from liquid state

Nguyen To Nga (1), Vo Van Hoang (2), Nguyen Hoang Giang (2)

(1) Faculty of Fundamental Science, PetroVietnam University; (2) Comp. Phys. Lab, HoChiMinh City Univ. of Technology, Vietnam National University - HoChiMinh City

Cooling rate effects on formation of 2D solid with square lattice structure from liquid state are studied by molecular dynamics (MD) simulation. The considered models consist of 6400 particles interacting via the square interatomic potential which is proposed by M. Rechtsman et al. (Phys. Rev. E 73, 011406 (2006)). Models are obtained by cooling from the melt at various cooling rates of 10^{-6}, 10^{-5} and 10^{-4} per MD step. Evolution of total energy per atom, specific heat, radial distribution function (RDF), and mean coordination number etc. is studied. Depending on the cooling rate used in simulation, crystallization or glass formation can occur. It is found that the crystallization of the 2D liquid with a square potential exhibits a first-order-like phase transition behavior. We find that main structural defects in the obtained 2D crystals are vacancies of various sizes and shapes, double triangles splitting from a strongly distorted square, rings of various sizes differed from 4-fold and distorted squares. Moreover, structure of the obtained 2D crystals is not homogeneous and it exhibits 'static heterogeneity', i.e. it contains clusters of atoms with different bond-orientation orders. Atomic mechanism of solidification of the system is studied via analysis of spatio-temporal arrangements of solid-like atoms occurred during the cooling process. Solidification occurs via homogeneous nucleation of nuclei of new phase and their subsequent growth following classical nucleation theory.

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Presenter: Nguyen To Nga

P.15 – Poster, NCTP-41

Diffusion of interstitial atoms in interstitial alloys FeSi and FeH with BCC structure under pressure

Nguyen Quang Học (1), Nguyen Thi Hoa (2), Dinh Quang Vinh (1) and Le Hong Viet (3)

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In our previous paper, the analytic expressions of the free energy of interstitial atom, the nearest neighbor distance between two interstitial atoms, the alloy parameters for interstitial atom, the diffusion quantities such as the jumping frequency of interstitial atom, the effective jumping length, the correlation factor, the diffusion coefficient and the activated energy together with the equation of state for the interstitial AB with BCC structure under pressure are derived from the statistical moment method. In this paper, we apply these theoretical results to interstitial FeSi and FeH in the interval of interstitial atom concentration from 0 to 5

Presenter: Nguyễn Thị Hòa

P.16 – Poster, NCTP-41

On the mass enhancement of black body background fluctuations

Nguyen Van Hoa (1), Le Van Xuan (2), Nguyen Tri Lan (3), and Nguyen Ai Viet (3)

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Motivated by the mass enhancement in the toy model of moving particle in Boltzmann and Gaussian background fluctuations, the contribution of black body background fluctuation to the effective mass of massless and massive particles is considered in this work. As the black body radiation depends only on its temperature, the dependence of the effective mass on temperature is obtained. The results, therefore, provides several physical insights for the research of complex systems where the interaction and equilibrium of a system and its surrounding are still not clear. By interpreting a characteristic parameter of the environmental contribution as its "effective temperature", "the thermal equilibrium" condition for complex systems would be discussed in the context of a thermodynamic theory.

Presenter: Le Van Xuan

P.17 – Poster, NCTP-41

Influence of the Confined Optical Phonon on the Radioelectric Effect in a Cylindrical Quantum Wire in the presence of Laser Radiation

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The influence of the confined optical phonons on the Radioelectric effect in a cylindrical quantum wire (CQW) subjected to a dc electric field, a linearly polarized electromagnetic wave and varying laser radiation, has been theoretically studied by using the quantum kinetic equation method. The analytical expression of the Radioelectric field (REF) is obtained as a function of the external electromagnetic waves energy, the temperature of the system, the wire's radius and especially the quantum numbers n, m which characterize the effect of phonon confinement. Numerical evaluations for the GaAs/AlAs cylindrical quantum wire show that the confined optical phonons enhance the probability of electron scattering, thus, lead to an increase of the REF when compared to the case of bulk phonons.

Presenter: Nguyen Quang Bau

P.18 – Poster, NCTP-41

Dynamical compactification of extra dimensions on the codimension 2-brane

Phan Hong Lien (1) and Do Thi Hong Hai (2)

(1) Le Quy Don Academy of Technology, 236 Hoang Quoc Viet, Hanoi, Vietnam; (2) Hanoi University of Mining and Geology, Duc Thang, Bac Tu Liem, Hanoi, Vietnam

We consider a codimension 2-brane moving in a warped dynamical six-dimensional space-time. The equations of motion of the brane and the anti-brane are derived to describe the cosmological evolution on the probe branes.

Presenter: Do Thi Hong Hai

P.19 – Poster, NCTP-41

Ideas about building a accelerator driven system (ADS) no target and uses thorium as a nuclear fuel

Tran Minh Tien

Thu Dau Mot University

Introducing the idea of using liquid lead which makes not only coolant but also target. So the target will not need to be replaced during nuclear reactor operation. The entire volume of liquid lead on the path of the incident proton beam in the ADSR (Accelerator Driven Subcritical Reactor) will be interactive target; therefore, the number of neutrons generated will increase in comparison with using conventional target. Providing preliminary calculations illustrating the above ideas.; discuss the possibility of using thorium as a nuclear fuel. Partly ideas were published in the article "Ability to make Accelerator-driven sub-critical reactor system (ADS) without target in (p, n) interaction - International Journal of Modern Physics and Application (2015)."

Presenter: Tran Minh Tien

P.20 – Poster, NCTP-41

Multiple Component Correlations in Quantum Mixtures of Ultracold Atoms

Nguyen Duong Bo and Tran Minh Tien

Institute of Physics, VAST, 10 Đào Tấn, Ba Đình, Hà nội, Việt nam

Quantum mixtures of ultracold atoms with multiple components are modeled by a multi-component Falicov-Kimball model. The model is analyzed using the dynamical mean field theory. A metal-insulator transition is observed in the homogeneous mixtures. It turns out that the metal-insulator transition occurs at both commensurate and incommensurate fillings. Ultracold atoms loaded in optical lattices give a great opportunity of studying fundamental problems related to strong correlation effects. The Mott transition was observed in fermionic atoms of K40. Recently, the research has been extended to multi-component fermionic atoms, in particular, the mixtures of K40 and Li6. The multi - component Hubbard model with both SU(3) and broken SU(3) symmetry repulsive interactions has been used to study the Mott transition. However, due to the mass imbalance of lithium and potassium atoms, a multi-component Falicov-Kimball model is more appropriate for studying the Mott transition in the mixtures.

Presenter: Nguyen Duong Bo

P.21 – Poster, NCTP-41

Magneto-thermoelectric effects in doped semiconductor superlattice in the presence of Laser radiation

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The magneto-thermoelectric effects in doped semiconductor superlattice (DSSL) in the presence of Laser radiation (LR) are studied with a periodical superlattice potential in the z-direction, subjected to a crossed electric field , magnetic field and LR characterized by electric field (where and are the amplitude and the frequency of the LR, respectively). The analytic expression for Ettingshausen coefficient (EC) is calculated by using the quantum kinetic equation for electrons.

The dependence of EC on the frequency, the amplitude of LR, the DSSL parameters and temperature gradient is obtained. The results are numerically calculated, plotted, and discussed for GaAs:Si/GaAs:Be DSSL to clearly show the dependence of EC in DSSL on the above values and parameters. Comparing with the results obtained in case of the bulk semiconductors, we see the differences because of the different structure, wave function and energy spectrum of DSSL. Keywords: Ettingshausen, Doped semiconductor superlatitice, Laser radiation, GaAs:Si/GaAs:Be

Presenter: Nguyen Quang Bau

P.22 – Poster, NCTP-41

Elastic deformation of binary and ternary interstitial alloy with FCC structure at zero pressure: Dependence on temperature, concentration of substitution atoms and concentration of interstitial atoms

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The analytic expressions of the free energy, the mean nearest neighbor distance between two atoms, the elastic moduli such as the Young modulus, the bulk modulus, the rigidity modulus and the elastic constants for interstitial alloy AC and interstitial alloy ABC (substitution alloy AB with interstitial atom C) with FCC structure at zero pressure are derived from the statistical moment method in previous paper. In this paper, we apply the general theoretical results. In this paper, we apply the theoretical results to the interstitial alloys AuLi and AuCuLi at zero pressure in different temperatures, concentrations of substitution atoms and interstitial atoms. Some calculated results for main metal in these alloys are compared with experiments and other calculations.

Presenter: Nguyễn Đức Hiền

P.23 – Poster, NCTP-41

A broadband laser-driven Kerr-like nonlinear coupler and entanglement

Doan Quoc Khoa (1), Cao Long Van (2), Nguyen Thi Dung (3), Le Thi Hoa (3), Nguyen Thi Thu (3) and Bui Van Dung (3)

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We present a model of Kerr-like nonlinear coupler, in which external coherent field is modeled by white noise. For such a system we derive a set of coupled stochastic integro-differential equations that can be averaged exactly. This result leads to some exactly analytical expression for the probability amplitudes of n-photon Fock states. In addition, we can see that the system is also able to generate Bell-like states and, as a consequence, the coupler discussed behaves as a two-qubit system. We also analyse the effects of dissipation on entanglement of formation parameterised by concurrence and compare these results with that obtained previously by other authors. As a interesting result, initially for a period of time the entanglement is enlarged when the chaotic parameter increases.

Presenter: Doan Quoc Khoa

P.24 – Poster, NCTP-41

Anisotropic Magnetism of PdCo Ultrathin Film: Density Functional Theory Study

Do Ngoc Son, Phan Thi Cam Giang*

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Conventional hard disk drives (HDD) use the in-plane magnetic recording technology. The maximum density of stored information is only 160 Gb/in2. Since the first generation of perpendicular magnetic recording HDD was realized in 2006, the high-density magnetic recording was established that is 500 Gb/in2 in 2010. It was predicted that the density of information can achieve up to 1.5 Tb/in2 before the perpendicular magnetic recording is replaced by more advanced technologies. The PdCo alloy is a good candidate for the perpendicular magnetic recording HDD. Therefore, we studied the perpendicular magnetic anisotropy of the PdCo alloy by using the density functional theory calculations. Electronic properties were analyzed to clarify the magnetic anisotropy of this alloy.

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Presenter: Do Son

P.25 – Poster, NCTP-41

Simple model for heating properties of protein-coated metallic nano-particles

Lương Thị Thêu (1), Trần Thị Nhàn (2), N. T. Lân (3), N. V. Thụ (1), N. A. Việt (3)

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The anomalous thermal denaturing of protein adsorbed to metallic nano-particles was observed in recent experiments and found a great application potential in bio-nano-technology and medical treatments. In this work, based on the Ginzburg-Landau phenomenological formalism we consider a new simple model to describe the heating properties of protein-coated metallic nano-particles. Using this proposed model, the temperature dependence of the maximum extinction as a function of temperature for BSA-coated gold nano-spheres was calculated. We found a further good agreement between the theoretical and experimental values

Presenter: Lương Thị Thêu

P.26 – Poster, NCTP-41

Suppression of Cardiac Alternans by Chaotic Attractors

Le Duy Manh (1), Pik-Yin Lai (2), C. K. Chan (3)

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To achieve control in dynamical systems, one usually avoids the generation of chaos. However, an effective control of an unstable dynamical system can also be practically achieved by deliberately inducing chaos in the system if the induced chaotic attractors are confined in a very small region in the phase space. Here, we reveal that the recently proposed T+T- control for cardiac alternans

suppression is due to the confined chaotic attractors mechanism by nonlinear dynamic analysis of the cardiac restitution model. These results are confirmed experimentally by detailed phase space portrait and transition dynamics measurements in whole heart experiments.

Presenter: Le Duy Manh

P.27 – Poster, NCTP-41

Higher-order nonclassical properties of nonlinear charge pair cat states

Dang Huu Dinh, Truong Minh Duc, and Tran Quang Dat

Center for Theoretical and Computational Physics, College of Education, Hue University, 34 Le Loi, Hue City, Viet Nam

We study the higher-order nonclassical properties of the nonlinear charge pair cat states. We show that these states exhibit antibunching to all orders and the antibunching exists depending on the variables, especially on the nonlinear functions. We also show that in such states, the higher-order squeezing appears only in the even orders and the degree of squeezing depends on the nonlinear functions.

Presenter: Trương Minh Đức

P.28 – Poster, NCTP-41

An application of q-deformed algebra to lattice vibrations

Nguyen Thi Ha Loan (1), Nguyen Tri Lan (2), Do Thi Thu Thuy (3), Hoang Hanh Phuong (4)

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The oscillator representation of quantum algebras has proved to be powerful for the study of the quantum optics, condensed matter physics, etc. In this paper we consider the possibility for the application of q-deformed algebra to lattice vibrations.

Presenter: Nguyen Thi Ha Loan

P.29 – Poster, NCTP-41

Theoretical model for plasmonic properties of graphene-based nanostructures

Do Chi Nghia (1) and Do Thi Nga (2)

(1) Hanoi Pedagogical University No.2; (2) Institute of Physics

In this work, we theoretically study the plasmonic properties of graphene on bulk substrates and graphene-coated nanoparticles. The surface plasmons of such systems are strongly dependent on bandgap and Fermi level of graphene that can be tunable by applying external fields or doping. An increase of bandgap prohibits the surface plasmon resonance for for GHz and THz frequency regime. While increasing the Fermi level enhances the absorption of the graphene-based nanostructures in these regions of wifi-waves. Some mechanisms for electric-wifi-signal energy conversion devices are proposed. Our results have a good agreement with experimental studies and can pave the way for designing state-of-the-art electric graphene-integrated nanodevices that operate in GHz-THz radiation.

Presenter: Do Chi Nghia

P.30 – Poster, NCTP-41

The simplest 3-3-1 model

L. T. Hue (1), L. D. Ninh (2), D. T. Huong (1), and T. D. Tham (3)

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A simple extension of the Standard Model (SM), based on the gauge group SU(3)C x SU(3)L x U(1)Y with Y being the hypercharge, is considered. We show that, by imposing an approximate global SU(2)L x SU(2)R custodial symmetry at the SM energy scale, the Z - Z' mixing is absent at tree level. Tree-level flavor-changing neutral currents (FCNCs) are also reduced to three particles, namely Z', a CP-odd Higgs and a CP-even Higgs.

Presenter: Le Tho Hue

P.31 – Poster, NCTP-41

Structure and dynamics of liquid Al2O3.2(SiO2) system as studied by Molecular Dynamics Simulation

Nguyen Van Yen (1), Nguyen Van Hong (1), Le The Vinh (2)

(1) Hanoi University of Science and Technology; (2) University of Ton Duc Thang

MD simulation using the Born-Mayer-Huggins type pairwise potential has been used to calculate the structure and properties for the liquid Al2O3-2SiO2(AS2) system. With in a 2000-5000 K temperature range at ambient pressure, the microstructure and dynamics of liquid AS2 system analysed through radial distribution function, bond angle distributions and coordination number distribution. The results show that, the short-range order (SRO) exists TOx(T is Si, Pb and x = 3-5). The intermediate range order(IRO) are also investigated in detail, it been show that have OTn(n = 2-4) linkages, between two adjacent TOx units connected via O atom common(corner-, edge-, and face-sharing). Besides, the visualization techniques was also used to clarify local structure of the models.

Presenter: Nguyen Van Yen

P.32 – Poster, NCTP-41

Evaluation the validity of the weak-field-approximation methods in consideration of the ionization rate of atoms

Nguyen Phuc (1), Pham Nguyen Thanh Vinh (2)

(1) Ho Chi Minh University of Science (2) Ho Chi Minh University of Pedagogy

Recently there are several theories used to investigate the ionization rate of atoms under the influence of the electric field have been proposed. These theories provide analytical formulae to quickly calculate the ionization rate of atoms for a wide range of field strength from tunneling to over-the-barrier regimes. However, the validity of them is still under debate. In this work, we provide a reliable tool based on Siegert-state method to generally evaluate the applicability of these approximation theories. Based on this evaluation, we can be able to utilize the best approximation approach with respect to the strength of the electric field. The limitation of each analytical formula is also discussed.

Presenter: Pham Nguyen Thanh Vinh

P.33 – Poster, NCTP-41

Optical cold atom trap with off-plane surface plasmon polaritons effect

Nguyen Thi Phuong Lan (1), Do Thi Nga (2), Nguyen Ai Viet (2)

(1) Hanoi Pedagogical University 2; (3) Institute of Physics, VAST

In-plane (parallel) and off-plane (orthogonal) surface plasmon polaritons at the interfaces between the dielectric and thin metallic film was studied. For the half-space (planar) geometry with ordinary in-plane surface plasmon polariton modes, the Kretschmann or Otto configurations are needed to create surface plasmons. In the case of thin metallic films with the thickness much smaller than the wave-length of excited laser beam, there are two modes of surface plasmon polaritons appeared: in-plane and off-plane. The off-plane surface plasmon polaritons do not need the additional configurations as in-plane case, and has weak dependence on the incident angle. In this work a possible application of off-plane for design optical cold atom traps was considered.

Presenter: Nguyen Thi Phuong Lan

P.34 – Poster, NCTP-41

Molecular Dynamics Simulation of Rutile – Anatase Heterojunction

Ca Nguyen Anh Khoa and Huynh Anh Huy

Can Tho University

In our research, the structure of heterojunction between anatase (100) and rutile (100) surface in monolayer and multilayer models are studied by Density Functional theory based on Tight-Binding method (DFTB). The near coincidence site lattice (NCSL) theory used to construct initial models. The interfaces have been annealed from 0K to 2250K in the linear ramp of 10ps, held there in 5ps and cooled back to 0K with an exponential ramp of 15ps. Interface structures have been investigated via the partial radial distribution functions, coordination number distributions, bond-angle distributions and interatomic distances. We found that both structures have the slightly disorder at the four-coordinate Ti atoms, band offset of rutile phase are 0.45eV in the conduction band and 0.51eV in the valence band higher than anatase ones. Electrons move from rutile to anatase, while holes move in the opposite direction.

Presenter: Ca Nguyễn Anh Khoa

P.35 – Poster, NCTP-41

Precise calculations of average level spacing in even - even nuclei

Le Thi Quynh Huong (1,2), Nguyen Quang Hung (3)

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Average level spacing at the neutron binding energy in even – even nuclei (numbers of neutrons and protons are both even) are calculated based on the precise calculations of nuclear level density (NLD) at given total angular momentum J and excitation energy E^*. The theoretical model used for the calculation is the Bardeen-Cooper-Schrieffer (BCS) theory at finite temperature and angular momentum, which describes the superfluid properties of hot rotating nuclei.

The results of average level spacing obtained within our theoretical model are closer to the experimental data than those obtained within previous theoretical approaches, which employed the approximate formula of the angular-momentum dependent NLD.

Presenter: Huong Thi Quynh Le

P.36 – Poster, NCTP-41

Carbo principle of maximum quantum similarity and application in stock exchange markets

Chu Thuy Anh, Nguyen Tri Lan, Nguyen Ai Viet

Institute of Physics, Hanoi

The transition from Boltzmann to Gaussian form of return distribution functions of stock exchange markets are well known and wildly investigated. Both Boltzmann and Gaussian distributions are the probability density functions with maximum entropy. Using the Carbo principle of maximum of quantum similarity we can find a one-one correspondence between the parameters of these distributions. Assume that the return distribution function of a stock exchange markets in the initial moment has Boltzmann-like form with certain parameters, at some time moment it changes to Gaussian-like probability density function satisfying the Carbo maximum principle of quantum similarity. We show that, by analyzing the height change of the return distribution functions in that time interval and using the uncertainty relations, we can define effective temperature, viscosity and their gradients of stock exchange markets.

Presenter: Chu Thuy Anh

P.37 – Poster, NCTP-41

Numerical solution of mean field theory for the three-component Ginzburg-Landau functional

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In a previous work, we have established the multi-component Ginzburg-Landau functional describing the correlation among the order parameters. At the same time we also obtained a selfconsistent system of equations which describes many-body relations between the physical quantities of the system where many kinds of fluctuations of corresponding order parameters are considered. To continue, in this work, we will try to carry out step by step numerical solution in order to show clear the relationships between the order parameters and their concrete contribution in processes. Numerical results would be presented in graphical evidence to illustrate the coexistence of many phases in many-body system.

Presenter: Nguyen Van Hinh

P.38 – Poster, NCTP-41

Energy spectrum inverse problem of q-deformed harmonic oscillator and entanglement of composite bosons

Nguyen Anh Sang, Do Thi Thu Thuy, Nguyen Thi Ha Loan, Nguyen Tri Lan, Nguyen Ai Viet

Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Thu Le, Ba Dinh, Ha Noi, Vietnam

Energy spectrum inverse problem was investigated in our previous work [1] using the connection between q-deformed harmonic oscillator and Morse-like aharmonic potential. We have proposed deformed-three-levels simple model, where the set-parameters of Morse potential and the corresponding set-parameters of level deformations are easily and explicitly defined. In this work, using this deformed-three-levels simple model we study the entanglement in composite bosons. Introducing the definition of relative entanglement (differential) entropy for composite bosons, we study the deformation of energy levels of a single boson when the surrounding environment effect was taken into account. Like the case of Fucault pendulum in experimental demonstration the rotation of the Earth, our deformation energy level investigation might be useful in detecting entanglement information of the system in a closed box and outside environment. Some application examples of our model are considered.

Presenter: Sang Anh Nguyen

P.39 – Poster, NCTP-41

The electroweak theory based on SU(4)L X U(1)X gauge group

H. N. Long (1), L. T. Hue (1), and D. V. Loi (1, 2)

(1) Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi, Vietnam; (2) Physics Division, Mathematics-Physics-Informatics faculty, Tay Bac University, SonLa, Vietnam

In the work, the first we present generalized gauge models based on SU(3)C X SU(4)L X U(1)X (3-4-1) gauge group with arbitrary electric charge of leptons. The mixing matrix of neutral gauge bosons is analysed, the eigenmasses and eigenstates are obtained. The anomaly free as well asmatching conditions are discussed precisely. In the second part, we present new development of the original 3-4-1 model. In difference from previous works, in this paper the neutrinos, with the help of the decuplet H, get the Dirac masses at the tree level. In the limit of lepton number conservation, the Higgs sector contains all massless Goldstone bosons for massive gauge bosons and the SM-like Higgs. Some phenomenology are pointed out.

Presenter: Duong Van Loi

P.40 – Poster, NCTP-41

A minimal 3-3-1 model for dark matter

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We show that the 3-3-1 model with minimal lepton content can work with only two scalar triplets, η and χ, while it leaves another scalar triplet, ρ' as an inert field, responsible for dark matter. The dark matter candidate is identified as the real or imaginary part of the second component of ρ'. We calculate the dark matter density and compare it with the data. We also make direct and indirect searches for the candidate under the light of the recent, new experiments.

Presenter: Le Duc Thien

P.41 – Poster, NCTP-41

Sequence dependent aggregation of peptides and fibril growth

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We study the aggregation of peptides in the tube model of proteins with hydrophobic-polar (HP) amino acid sequences and correlated side chain orientations for hydrophobic interaction. Monte Carlo simulations are carried out to calculate equilibrium and dynamic properties of systems of different numbers of peptides and for various sequences of length of 8 amino acids. It is shown that the aggregation propensity as well as the structures of aggregates are strongly dependent on the amino acid sequence and the number of peptides. At a presumable physiological temperature, aggregation is observed not for all but several sequences. Among the sequences studied, only one leads to a fibril-like β-sheet structure. The fibril growth depends on peptide concentration and is consistent with the nucleation and growth mechanism. The time dependence of the number of fibril-forming peptides is essentially exponential at low temperatures, and it becomes sigmoidal near the aggregation transition temperature. Strikingly, a binary mixing of peptides with fibril prone and non-fibril prone sequences shows conversion of the latter to fibrillar structure.

Presenter: Nguyen Ba Hung

P.42 – Poster, NCTP-41

Network structure of SiO2 and MgSiO3 in amorphous and liquid States

Nguyen Van Hong, Tran Thuy Duong, and Mai Thi Lan

Đại học Bách khoa Hà Nội

Network structure of SiO2 and MgSiO3 at 300 K and 3200 K is invetsigate by molecular dynamics simulation and visualization of simulation data. Structural organization of SiO2 and MgSiO3 is clarified via analysising the short range order (SRO) and intermidiate range order (IRO). Network topology is determined via analysing the bond between structural units, the cluster of structural units as well as spatial distribution of structural units. The polyamorphism and dynamic heterogeneity are also discussed in this work.

Presenter: Nguyễn Văn Hồng

P.43 – Poster, NCTP-41

Atomic structure of nanometer-sized amorphous TiO_2

Phan Thanh Hung (1), Le Thi Hong Diep (2), Le Thi Cam Loan (1), Huynh Anh Huy (2)

(1) Tra Vinh University (2) Can Tho University

TiO_2 nanoparticles with different configuration and size from 0.8 nm to 2.7 nm in anatase and rutile phases are studied by Density Functional theory based on Tight-Binding (DFTB). The structure and properties of amorphous TiO_2 greatly depend on their size. The surface energies are calculated to provide useful instructions to the fabrication of TiO_2 nanoparticles.

Presenter: Phan Thanh Hùng

P.44 – Poster, NCTP-41

Growth of graphene by vapor deposition method and size effects on its structure.

Nguyen Hoang Giang (1), Vo Van Hoang (1), Le Nhu Ngoc (2)

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We report MD simulation of growth of graphene by vapor deposition on BN. The systems (containing carbon vapor and BN substrate) are relaxed at high temperature (1500 K) then it cooling down to room one (300 K. Surface atoms interact with substrate via Lennard-Jones potential while the interaction between carbon atoms is computed via Tersoff potential. Depending on the size, different crystalline honeycomb structures have been found. Structural properties of the graphene obtained at 300K are studies by analyzing radial distribution function (RDF), coordination number, ring statistics, interatomic distance, bond-angle distribution and 2D visualization of atomic configurations. We find that although two models containing various numbers of atoms have a honeycomb structure, differences in structural properties of graphene formed by vapor deposition on substrate and free standing one can be found. Moreover, size effects on structure are significant.

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Presenter: Nguyen Hoang Giang

P.45 – Poster, NCTP-41

Melting Boron Nitride Nanoribbons

Nguyen Thi Thuy Hang

Ho Chi Minh City University of Technology.

Melting of hexagonal Boron Nitride (BN) model in 2D space is studied via molecular dynamics simulation. The model contains 10000 atoms interacted via long-range bond-order potential (LCBOP). Model is heated up from 50 K to 7000 K in order to see the melting rate dependence of various thermodynamic quantities, structural characteristics, occurrence of various structural defects upon heating to a molten state. Some thermodynamic quantities are presented: Temperature dependence of total energy exhibits a first-order-like behavior of the transition at a melting point; heat capacity of the system exhibits a single peak at around the melting point. Melting point of hexagonal Boron Nitride (BN) in 2D space is rather high due to constraint of the 2D space.

Presenter: Nguyen Hang

P.46 – Poster, NCTP-41

Uphill diffusion of vacancy in boron diffusion process in silicon

Vu Ba Dung

Hanoi University of Mining and Geology, Vietnam

Uphill diffusion is an interesting phenomenon, in which diffusion flux goes to higher concentration area (goes uphill). Uphill diffusion had been found and studied since 1949. A number of different approaches have been proposed for treatment of uphill diffusion. Most of researching about uphill

diffusion showed that: uphill diffusion occurs in muticomponent systems and diffusion flux of a component is strongly coupled to its partner species that is cause of uphill diffusion. In this paper, uphill diffusion of vacancy in simultaneous diffusion of boron and point defect in silicon is presented and discussed. Results showed that: Vacancy can diffuse uphill in simultaneous diffusion in silicon; cause of uphill diffusion can be the coupled effect of vacancy diffusion fluxes with boron flux and/or direct interaction between boron molecules and vacancies.

Presenter: Vu Ba Dung

P.47 – Poster, NCTP-41

Lepton flavor violating decay of neutral Higgs in seesaw models

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The lepton flavor violating decay of the Standard Model-like Higgs (LFVHD) is discussed in seesaw models at the one-loop level. Being different from all previous works, the unitary gauge is used for computing the LFVHD processes and compare with the LFVHD results reported recently.

Presenter: Nguyễn Huy Thảo

P.48 – Poster, NCTP-41

On the concentration dependence of metallic nano-particles in enhanced Forster resonance energy transfer

Nguyen Minh Hoa (1), Chu Viet Ha (2), Dinh Thi Thuy (3), Nguyen Tri Lan (4), Tran Hong Nhung (4), Nguyen Ai Viet (4)

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The enhanced Forster resonance energy transfer is obtained in recent experiments. One of most important experimental fact is the observed strong enhance of donor fluorescence with increasing the concentration of metallic nano-particle acceptors in the first stage. We propose three types of energy transfer mechanisms (Forster FRET, surface SET and Coulomb CET) and predict simple relations for their dependences on the concentration of metallic nano-particles. The competition of these mechanisms leads to the transfer intensity dependence on the concentration dependence of metallic nano-particles. Using these assumptions, we obtain quite good agreement of the theoretical results with experimental data.

Presenter: Nguyễn Minh Hoa

P.49 – Poster, NCTP-41

The spatially anisotropic triangular lattice antiferromagnet: Popov-Fedotov method

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We present an analysic of the antiferomagnetic Heisenberg model on an triangular lattice with spatially anisotropic J1-J2 exchange interactions. We apply the Popov-Fedotov method based on introducing an imaginary valued chemical potential to enforce the auxiliary fermion constraint exactly. The staggered magnetization, magnon spectra, the ground state energy are computed in one loop approximation and compared using two different constraints: exact and on average. In the limit of zero temperature the results are identical, whereas at higher temperature significant differences are found: The comparisons with the results obtained by other methods are discussed.

Presenter: Pham Thi Thanh Nga

P.50 – Poster, NCTP-41

Thermodynamic property of interstitial alloy FeSi with vacancy and BCC structure: Dependence on temperature, concentration of interstitial atoms and concentration of equilibrium vacancies

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The analytic expressions for the concentration of equilibrium vacancies and the thermodynamic quantities such as the mean nearest neighbor distance, the free energy, the isothermal and adiabatic compressibilities, the isothermal and adiabatic elastic modulus, the thermal expansion coefficient, the heat capacities at constant volume and at constant pressure, the entropy of binary interstitial alloy with defect and with body-centered cubic (BCC) structure with the concentration of interstitial atoms is small (below 5%) are derived by the statistical moment method. The obtained expressions of these quantities depend on temperature, concentration of interstitial atoms and concentration of equilibrium vacancies. The theoretical results are applied to interstitial alloy FeSi in the interval of temperature from 600 to 1000K and in the interval of interstitial atom concentration from 0 to 5%. In the case when the concentration of interstitial atoms Si is equal to zero, we obtain the thermodynamic quantities of main metal Fe with defect. Our calculated results for the thermal expansion coefficient and the heat capacity under constant pressure of main metal Fe are in good agreement with experiments. Our results show that the concentration of equilibrium vacancies affect thermodynamic property of interstitial alloy in high temperatures.

Presenter: Nguyễn Thị Hòa

P.51 – Poster, NCTP-41

Charge Creation from Extra Dimensions

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This is an extended version of the work recently published (DVDuc and NMGiao, Int. J. Theor.

Phys. vol 55, p. 959, 2016), where a mechanism has been proposed for explaining the originality of charge creation based on some specific assumptions related to space-time extra dimensions. It holds that the existence and the compactification of extra dimensions are the origin for creating the interaction charge in ordinary 4-dimensional space-time.

Presenter: Dao Vong Duc

P.52 – Poster, NCTP-41

Single-active-electron model potential for a polar molecule CO

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In recent experiments, the permanent dipole and the core dynamics have been identified to play an important role in the strong-field high-order harmonic generation (HHG) of polar molecules such as CO. For the purpose explaining the effects theoretically, we develop an ab initio methods for calculating HHG for polar molecules by numerically solving the time-dependent Schrodinger equation within the single-active-electron (SAE) approximation. In this brief report, we show how to construct a three-dimensional SAE model potential for a polar molecule CO. In first step, the molecular wave function calculated by the DFT method implemented in GAUSSIAN program is used for construction of SAE model potential in the zero-th approximation order. Because the GAUSSIAN wave functions are not good in the asymptotic region, the obtained model potential in this region is needed to be corrected by fitting it with the Coulomb potential. Our SAE model potential of CO well agrees to other theoretical calculations, but for our requirement of accuracy, we are going to apply one more iteration in order to get the more accurate SAE model potential. The next step is to calculate the HHG of a polar molecule CO with and without consideration of the molecular core dynamics, and then to study the effects of the core dynamics and the permanent dipole on the HHG spectra.

Presenter: Trần Lan Phương

P.53 – Poster, NCTP-41

Phase diagram of hydrophobic thick ribbons

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A ribbon is an intermediate object between a polymer and a membrane, which is frequently found in everyday life, in biology and in nanotechnology. We study the ground state phase diagram of a thick ribbon with hydrophobic surface as a function of the length of the ribbon and the diameter of solvent molecule. It is assumed that the ribbon can adopt several configurations including a globule, a rolled, a curled, a helix and a twisted conformation as its ground state. It is shown that the ribbon's non-zero thickness leads to a broken rotational symmetry of the ground state conformation. Analytical calculation supported by Monte Carlo simulations shows favorable ribbon configurations for different solvent sizes including a striking appearance of the twisted configuration even in absence of any intrinsic chiral potential. Our description of DNA as a twisted thick ribbon may serve as a useful model for DNA binding.

Presenter: Trịnh Xuân Hoàng

P.54 – Poster, NCTP-41

Melting temperature and thermo-mechanical properties of iron in Debye model

Nguyen Thi Thu Hang (1), Phung Thi Lan (1), Tran Thi Hai (1), and Ho Khac Hieu (2)

(1) Hong Duc University, Thanhhoa, Vietnam; (2) Duy Tan University, Danang, Vietnam

The pressure effects on thermodynamic properties of iron have been studied based on the semi-empirical approach in the Debye model. The recent well-established pressure-dependent Grüneisen parameter has been applied to derive the analytical expressions of the Debye frequency, the Debye temperature, the melting temperature and the shear modulus as functions of pressure. The values of these quantities at zero pressure are evaluated using the anharmonic correlated Debye model. Numerical calculations have been performed for ϵ-iron up to volume compressibility 0.6 and the corresponding pressure. Theoretical calculations are compared with those of experimental data showing the good and reasonable agreements.

Presenter: Ho Khac Hieu

P.55 – Poster, NCTP-41

Influence of phonon confinement on the nonlinear optically detected electrophonon resonance linewidth in parabolic quantum wells

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We investigate the influence of optical phonon confinement described by Huang-Zhu model on the nonlinear optically detected electrophonon resonance (NLODEPR) effect and NLODEPR linewidth in parabolic quantum wells by using the operator projection. The obtained numerical result for the GaAs/AlAs parabolic quantum well shows that the NLODEPR linewidths depend on the confinement frequency and temperature. Besides, in the two cases of confined and bulk phonons, the linewidth (LW) increases with the increase of temperature and confinement frequency. Furthermore, in the large range of the confinement frequency, the influence of phonon confinement plays an important role and cannot be neglected in considering the NLODEPR linewidth.

Presenter: Tran Cong Phong

P.56 – Poster, NCTP-41

Structural properties of amorphous 2D solid from the Liquid State with Square Potential

Nguyen To Nga (1), Vo Van Hoang (2), Nguyen Hoang Giang (2)

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Structural properties of amorphous 2D solid with distorted square lattice-like structure from the liquid state is studied by molecular dynamics (MD) simulation. Models contain 6400 particles interacted via the square interatomic potential proposed by M. Rechtsman et al. (Phys. Rev. E 73, 011406 (2006)). Structure of amorphous 2D solid formed by cooling from the melt is inves-

tigated by analyzing the radial distribution function (RDF), coordination number distribution, ring statistics, bond – orientation order, interatomic distance and bond-angle distributions, visualization of atomic configurations. Main structural defects found in the obtained 2D solid are vacancies of different sizes and shapes such as double triangles splitting from a distorted square, rings of various sizes and distorted squares. Discovery of 2D iron with a square lattice structure suspended in pores of graphene sheet by experiment (J. Zhao et al., Science 343, 1228 (2014)) has stimulated the researches related to 2D iron and other 2D metals by both experiments and computer simulations in general. However, our understanding of structure and thermodynamics of 2D iron is completely lacking since main attention has focused on its thermal stability, magnetic behaviors and/or possibility of applications in practice. Therefore, our MD simulation of the formation of amorphous 2D solid from the liquid with square potential provides additional information for understanding of structure of amorphous 2D iron.

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Presenter: Nguyen To Nga

P.57 – Poster, NCTP-41

Investigation of the nonsequential process of helium induced by two-color laser pulses

Huynh Van Son (1), Truong Dang Hoai Thu (2), Tran Hoang Hai Yen (3), Pham Nguyen Thanh Vinh (2)

(1) Ho Chi Minh University of Science; (2) Ho Chi Minh University of Pedagogy; (3) Sai Gon University

In this study, the nonsequential process of helium induced by two-color laser pulses consisting of 800-nm and 400-nm fields is investigated using full three-dimensional classical ensemble model. We consider situations where two components of the pulse are orthogonal and in parallel to each other. By tuning the relative phase of the laser pulses, the correlated dynamics between two ionized electrons can be strongly modified. Trajectory analysis indicates that the roots of this modification in electronic correlated dynamics are the instant of double ionization, the repulsive force between two ionized electrons, and the energy sharing dynamics between them toward the recollision process. The dependence of He^{2+} yield on the relative phase of the pulses is also discussed.

Presenter: Truong Dang Hoai Thu

P.58 – Poster, NCTP-41

Study of crystallization mechanisms of Fe nanoparticle

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Fe nanoparticles (NP) were investigated by means of molecular dynamics simulation. The crystallization mechanisms was studied through the time evolution of crystal cluster and potential energies of different types atoms. The simulation shows that the NP was crystallized into bcc crystal structure when it was annealed at 900 K for long times. Analyzing the energies of differ-

ent type atoms, we found that the crystal growth is originated from specific atomic arrangement in the boundary region of crystal clusters. Further study concerns the morphologies of NP. It was shown that different morphologies differ strongly not only in the core, but also in the surface of NP. Unlike amorphous NP, the structural organization of phases in the crystalline sample is more complicated and cannot be described by simple shell/core model.

Presenter: Giap Thuy Trang

P.59 – Poster, NCTP-41

Measurement of entanglement degree and controlled teleportation in the trio coherent states

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In this paper, we measure the entanglement degree of the trio coherent states by using the linear entropy criterion. It is proved that the degree of intermodal entanglement in these states becomes more pronounced when increasing the parameter r. When using these states as an entanglement resource to control the teleportation a state, the degree of average fidelity of controlled teleportation process becomes bigger and bigger by increasing the correlative parameter r.

Presenter: Trương Minh Đức

P.60 – Poster, NCTP-41

Negatively charged excitonin the atomic monolayer with the presence of a magnetic field

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Recently, the measurement of binding energy of excitons in the two-dimensional physics systems such as graphene or transition-metal dichalcogenides (TMDs) is of great interest. In this work, the FK operator method combined with the Laplace transformation is used to calculate the energy spectra of the negatively charged exciton in atomic monolayers with the presence of a magnetic field. The obtained results are well compared with the other numerical methods and will be used for analyzing some experiments carried out for the considered system. Particularly, the magnetic enhancement of the screening effect for the Coulomb interaction in the TMD monolayer WS2 will be investigated.

Presenter: Nguyễn Phương Duy Anh

P.61 – Poster, NCTP-41

On the theory of three types of polaritons (phonon, exciton and surface plasmon polaritons)

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We analyze and compare three well-known types of polaritons: phonon polariton, exciton polariton and surface plasmon polariton. For first two types (phonon polariton and exciton polariton) the interaction between photon and media can be expressed via a longitudinal-transversal splitting (LT-splitting), while for third type of polariton (surface plasmon polariton) via the boundary condition. Considering the existence of an analogy picture of these three types of polaritons, an effective LT-splitting was introduced for surface plasmon polariton. The Nambu broken symmetry theory and Anderson-Higgs mechanism are discussed for lower branch of these polaritons.

Presenter: Duong Thi Ha

P.62 – Poster, NCTP-41

Influence of an External Magnetic Field on the Acoustomagnetoelectric Field in a Cylindrical Quantum Wire with a Parabolic Potential

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The acoustomagnetoelectric (AME) field in a cylindrical quantum wire with a parabolic potential (CQWPP) is theoretically investigated in the presence of an external magnetic field (EMF) by using the quantum kinetic equation for the distribution function of electrons scattering with internal acoustic phonon and electrons system interacting with external phonons in a CQWPP. The analytic expression for the AME field in the CQWPP in the presence of the EMF is obtained. The dependence of AME field on the frequency of external acoustic wave, the cyclotron frequency of the EMF and the intensity of the EMF is achieved. Theoretical results for the AME field are numerically evaluated, plotted and discussed for a specific CQWPP GaAs/GaAsAl. This result has shown that the dependence of the AME field on intensity of the EMF is many distinct maxima in the quantized magnetic region. These results also compared received fields with those for normal bulk semiconductors, quantum well and quantum wire to show the difference. The influence of an EMF on AME field in a CQWPP is newly developed.

Presenter: Nguyen Van Nghia

P.63 – Poster, NCTP-41

Effects of phonons in the excitonic insulator in the 2D extended Falicov-Kimball model

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Excitonic insulator instability in the 2D extended Falicov-Kimball model at zero temperature has been investigated when a coupling of electrons and vibrational degrees of freedom is taken into account. Adopting the unrestricted Hartree-Fock approximation, both electron-phonon interac-

tion and electron-electron interaction are treated in an equal footing. Numerical results show us that the excitonic insulator coexists with the lattice displacement only if the electron-phonon coupling is large enough. At a given small electron-phonon coupling, one finds a stability of excitonic insulator only in between two critical points of the electron-electron interaction strength. Detail ground state phase diagrams of the excitonic-insulator in the model then are presented and discussed.

Presenter: Do Thi Hong Hai

P.64 – Poster, NCTP-41

The orientation dependence of high-order harmonic generation and ionization probability of H2+ considering the nuclear vibration

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We investigate the dependence on the molecular orientation of high-order harmonic generation (HHG) and ionization probability by numerically solving the time-dependent Schrödinger equation of vibrating molecule exposed to an intense laser pulse. The results show that with nuclear motion, the intensity of HHG spectrum is minimized at the harmonic order less than that in case of fixed nuclear. The stronger the nuclei vibrate, the higher the orientation angle of the minimum is. Besides, the HHG intensity undergoes a minimum with increasing the orientation angle. In addition, at this "critical orientation angle", the phase of harmonic of vibrating molecule undergoes a jump by about Pi radian. The ionization probability decreases with increasing the orientation angle.

Presenter: Phan Thi Ngoc Loan

P.65 – Poster, NCTP-41

Controllable electronics structure in Zigzag Bilayer Graphene nanoribbons

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Graphene, consisting of one or a few crystalline monolayers of carbon atoms, stands out because of its electronic properties for applications in nanoelectronics. However, this material also suffers from a strong drawback for most electronic devices due to the gapless character of its band structure, which makes it difficult to switch off the current. In our model, we propose a method to control the gap. We use a transverse electric field generated by side gates and a vertical electric field generated by top/back gates to modulate the band gap and investigate the electronic structure of Zigzag Bilayer Graphene nanoribbons (Bernal stacking) based on the Tight Binding calculation method. The band structure of Zigzag Bilayer Graphene has flat bands, which appear in the range of 2pi/3 - pi . Under the effects of an external electric field, the gap is opened depending on its value. Specifically, in this case, the gap will be changed most when U is in the range of [0.5V, 1.5V]. Comparing the electric fields perpendicular to parallel the difference was found to be larger in the parallel field, but the arranging order of the charged particles was changed to a greater amount in the shape of band structure of Zigzag Bilayer Graphene

nanoribbons. More importantly, the value of the bandgap is largest under simultaneous effects of the two fields. Then, our group continued to examine the effects on transmission and Seebeck coefficients to control their physical properties under electric fields. So, thanks to the application of external electric fields, we can open and control the gap of Zigzag Bilayer Graphene nanoribbons . We believe that our results highlight a promising direction for Graphene-based semiconductors that can be used to create new electronic devices with a high on/off current ratio.

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Presenter: Nguyen Thi Kim Quyen

P.66 – Poster, NCTP-41

A non–extensive thermodynamic theory of ecological systems

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After almost 30 years of development, it is not controversial issue that the so–called Tsallis entropy provides a useful approach to studying the complexity where the non–additivity of the systems under consideration is frequently met. Also, in the ecological research, Tsallis entropy or in other words, q –entropy has been found itself as a generalized approach to define diversity indices including Shannon–Wiener and Simpson indices. As a further stage of development in theoretical research, a thermodynamic theory based on Tsallis entropy or diversity indices in ecology has to be constructed for ecological systems to provide knowledge of ecological macroscopic behaviors. The standard method of theoretical physics is used in the manipulation and the equivalence between phenomenological thermodynamics and ecological aspects is the purpose of the ongoing research.

Presenter: Le Van Xuan

P.67 – Poster, NCTP-41

Theoretical studies of energy band structure and density of state of Penta-Graphene

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Recently, a new carbon allotrope has been proposed, similar to graphene, which is called penta-graphene. State of the art theoretical calculations confirm that penta-graphene is a semiconductor and possesses an intrinsic quasi-direct band gap as large as 3.25 eV. In this paper, we use the tight-binding method to discuss about band structure and present an analytical solution to examine the band evolution of penta-graphene. We compare with the resulting band gap of penta-graphene when calculated by using HSE06 function, this shows that the suitable tight-binding hopping parameter is t=4.3623 and only one fitting is involved by choosing t'/t=0.2. This result shows feasibility in our models and also is the basis for subsequent studies. To probe

the electronic properties of penta-graphene, we incorporate the use of the Green's functions formalism to calculate density of state and transport characteristics of this material. The versatility of penta-graphene is expected to have broad applications in future, especially in nanoelectronics and nanomechanics. This reseach is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2015.98

Presenter: Pham Thanh Thuy

P.68 – Poster, NCTP-41

Nuclear reactor calculations using MCNP6 code based on a CAD model

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In this paper, a new MCNP6 model of the Training Reactor of Budapest University of Technology and Economics (BME) was developed by using SuperMC, a CAD-based Monte Carlo method for integrated simulation of nuclear systems by making use of hybrid and deterministic methods and advanced computer technologies. We calculate some physical parameters of BME reactor as total effective multiplication factor with different control rod positions, with various water levels and temperatures of water; delayed neutron fraction and neutron flux distribution. Comparison of the calculated results with experimental data were also done.

Presenter: Nguyen Ba Vu Chinh

P.69 – Poster, NCTP-41

Simple model for dielectric constant of water at low frequencies

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Dielectric constant of liquid water still is poorly understood, in particular at low frequencies, although it is very essential in understanding the dynamics, stability and flexibility of biomolecules. Recently, the dielectric constant of water at low frequency under 1 MHz and at different temperatures was measured. They have found that there is a very special frequency called the isopermitive point where the value of dielectric constant is independent of temperature. The dielectric constant of water decreases above this point, and increases below it with increasing temperature. This point might plays the same important role in living systems like the isosbestic point in chemical reactions or Raman spectroscopy. We propose a simple theoretical model for the dielectric constant of water at low frequencies where liquid water are considered as a plasma with two charge species: ions and dipoles. Our simple model found a good agreement between the theoretical and experimental data, and could be useful for further investigation the relation processes and biological behavior of live cells around the special crossing points.

Presenter: Tran Thi Nhan

P.70 – Poster, NCTP-41

Metal-insulator transition in the standard three-component Falicov-Kimball model

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The standard three-component extension of the spinless Falicov-Kimball is studied within the dynamical mean-field theory. The extended model consists of an itinerant single component and localized two components. The local Coulomb interaction between model components is also included. The homogeneous phase exhibits the correlation-induced metal-insulator transition. For SU(3) symmetry interaction the metal-insulator transition only occurs at commensurate fillings. For interactions with SU(3)-broken symmetry, the metal-insulator transition additionally occurs at incommensurate half filling.

Presenter: Nguyen Duong Bo

P.71 – Poster, NCTP-41

On the existence of graphene-like liquid water structure

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The intensive studies towards graphene have stimulated recently huge interests on graphene-like 2D layered nanomaterials. The relaxed crystalline water structure obtained from the modified ice *Ih* crystal symmetry shows $P_{6/mmc}$ space group sheet consisted of Oxygen atoms. The DFT calculations implemented by Abinit package show for Oxygen honeycomb lattice layer the O-O bond length of 2.612 Å, the lattice constant of 4.523 Å. The application of the graphene tight-binding model unveils the value of 2.71 eV absorption peak which is well-fitted with the experiment data.

Presenter: Le Tuan

P.72 – Poster, NCTP-41

Pressure-dependent structural heterogeneity in calcium silicate glass

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This work presents a molecular dynamics simulation of CaSiO3 glass using Born–Mayer–Huggins potentials. The structural organization and structural phase transition under compression as well as network structure of CaSiO3 are clarified through analysis and visualization of molecular dynamics simulation data. The short-range order structure, intermediate-range order structure and the degree of polymerization of SiOx-network are also discussed in detail.

Presenter: Mai Thi Lan

P.73 – Poster, NCTP-41

Electron-phonon resonance linewidth in triangular quantum well via two-photon absorption process

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Electron–phonon resonance linewidth in triangular quantum well is investigated via two–photon absorption process when electrons are scattered by longitudinal optical phonons (LO–phonons). Using the projection operator method, we obtain the expression of absorption power in the case of two–photon absorption. The dependence of absorption power on photon energy with different values of amplitude electric field, temperature and well width is indicated. The results are compared to those in the quantum well models with different types of confined potentials.

Presenter: Vinh Tuan Pham

P.74 – Poster, NCTP-41

Optical properties of Tamm states base on 1D Thue-Morse quasi-photonic crystals

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Using the invariant imbedding methed developed by us recently, we study optical properties of Tamm states base on 1D Thue-Morse quasi-photonic crystals. We find that there are many optical plasmon excitation states in absoption spectra in both Otto and Krestchmann configurations. The maximum of absorption peak and the number of absorption peak increase when the number layer of the quasi-photonic crystal increases. In some configurations the absorption peak is higher than the absorption peak of Tamm states base on 1D photonic crystals. We also find that the electromagnetic field between metal-dielectric interface is large enhanced in both Otto and Krestchmann configuration.

Presenter: Phung Duy Khuong

P.75 – Poster, NCTP-41

Influence of phonon confinement on the optically detected magneto-phonon resonance line-width in quantum wells

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We investigate the influence of phonon confinement on the optically-detected magneto-phonon resonance (ODMPR) effect and ODMPR line-width in parabolic quantum wells. The ODMPR conditions as functions of the well's parameters and the photon energy are also obtained. The shifts of ODMPR peaks caused by the confined phonon are discussed. The numerical result for a specific quantum well shows that in the two cases of confined and bulk phonons, the line-

width (LW) is sensitive for changing of the confinement frequency, doped concentration, and temperature. Furthermore, in the large range of the confinement frequency, the influence of phonon confinement plays an important role and cannot be neglected in reaching the ODMPR line- width.

Presenter: Nguyen Dinh Hien

P.76 – Poster, NCTP-41

Metal-insulator transitions in silicene with spin orbit-interaction

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We study a two-dimensional ionic Hubbard model with spin orbit interaction on a honeycomb lattice as a simple basis for describing the electronic structure of silicene in the presence of an electric field induced by the substrate. The local lattice Green function of the model is obtained within the coherent potential approximation. The influence of the spin orbit interaction on the Mott transition is investigated by the density of states at the fermi level and the energy gap. The critical values of correlation-driven metal–insulator transitions are estimated. Our results are closely relevant to current experimental and theoretical researches in silicence.

Presenter: Nguyen Thi Huong

P.77 – Poster, NCTP-41

Study on elastic deformation of AB substitution alloys with FCC structure at zero pressure

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The analytic expressions of the free energy, the mean nearest neighbor distance between two atoms, the elastic moduli such as the Young modulus, the bulk modulus, the rigidity modulus and the elastic constants for AB substitution alloy with FCC structure at zero pressure are derived from the statistical moment method in previous paper. In this paper, we apply the theoretical results to the substitution alloys AlCu, AlMg, AuCu, CuZn at zero pressure in different temperatures and concentrations of substitution atoms and some calculated results for main metals in substitution alloys are compared with experiments.

Presenter: Nguyễn Đức Hiền

P.78 – Poster, NCTP-41

Phenomenology of the 3-2-3-1 model

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In this work we study the details of the left-right asymmetry models based on SU(3)C X SU(2)L X SU(3)R X U(1)X gauge group. The gauge and Higgs mass spectrums are studied. All the interac-tions of the gauge bosons with the fermions and scalars are derived. We study a few $\Delta F = 2$ avor changing neutral current processes by considering the effects of both the neutral vectors $Z_{R\mu}$ and a new scalar Higgs. It leads to the strong constraint on the new physical scale, $M > 10^3$ - 10^4 TeV.

Presenter: Duong Van Loi

P.79 – Poster, NCTP-41

Thermodynamic property of binary interstitial alloy with FCC structure: Dependence on temperature and concentration of interstitial atoms

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The analytic expressions of the thermodynamic quantities such as the mean nearest neighbor distance, the free energy, the isothermal and adiabatic compressibilities, the isothermal and adiabatic elastic modulus, the thermal expansion coefficient, the heat capacities at constant volume and at constant pressure, the entropy of binary interstitial alloy with face-centered cubic (FCC) structure with the concentration of interstitial atoms is very small are derived by the statistical moment method. The obtained expressions of these quantities depend on temperature and concentration of interstitial atoms. The theoretical results are applied to interstitial alloy AuSi. In the case when the concentration of interstitial atoms is equal to zero, we obtain the thermodynamic quantities of main metal. Our calculated results for the thermal expansion coefficient and the heat capacity under constant pressure of main metal are in good agreement with experiments.

Presenter: Dinh Quang Vinh

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