Program & Abstracts

42nd National Conference on Theoretical Physics

HỘI NGHỊ VẬT LÝ LÝ THUYẾT TOÀN QUỐC LẦN THỨ 42

Cần Thơ

31 July - 3 August, 2017

Program & Abstracts

42nd National Conference on Theoretical Physics

Ninh Kieu Riverside Hotel
2 Hai Bà Trưng, Ninh Kiều
Cần Thơ, Việt Nam

31 July - 3 August, 2017

Contents

Welcome Message

It is my great pleasure to welcome you in the *42nd National Conference on Theoretical Physics* (NCTP-42) in Can Tho city.

The NCTP-42 is co-organized by the Institute of Physics – Vietnam Academy of Science and Technology (IOP-VAST) and Can Tho University (CTU) under the support of the Vietnam Theoretical Physics Society (VTPS).

The NCTP is an annual scientific forum dedicated to the dissemination of the latest developments in the field of theoretical physics. It has been organized annually for more than 40 years since the first time in 1976.

The mission of NCTP 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 123 participants from more than 30 research and educational institutions in Vietnam and in the region. Two invited talks, 25 oral and 80 poster contributions will be presented at the conference.

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

Nguyen Ai Viet
Institute of Physics, VAST
Chair of NCTP-42

Prof. Nguyen Ai Viet is currently the President of the Vietnamese Theoretical Physics Society.

Committees

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- Can Tho University (CTU)

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- Vietnam Academy of Science and Technology (VAST)

General Information

Conference Venue

The NCTP-42 conference takes place in:

Ninh Kieu Riverside Hotel (Ninh Kieu 1 Hotel)
2 Hai Ba Trung, Ninh Kieu
Can Tho, Vietnam.

Direction

The conference venue is 12 km from Can Tho International Airport (VCA), and can be reached from the airport in 25 min. by taxi.

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

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 Sapphire meeting room on the 3rd floor of Ninh Kieu Riverside Hotel.

Lunches

Lunches are provided for conference participants during 31 July - 2 August (3 days) in the hotel restaurant on the first floor of Ninh Kieu 1 Hotel. Lunch coupons are included in your name badge holder.

Gala Dinner

All participants are invited to the Gala Dinner.

Time: 31 July 2017, from 18:00 PM
Place: Du thuyền Ninh Kiều (Restaurant on the River Boat in front of Ninh Kieu 1 Hotel)

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

Excursion

All participants are invited to a Can Tho tour on the river. The tour program consists of visiting Cai Rang floating market (Chợ nổi Cái Răng), South Truc Lam Monastery (Thiền viện Trúc lâm Phương Nam), My Khanh tourist village (Làng du lịch Mỹ Khánh).

Time: 7:00 AM - 11:00 AM, Tuesday, 1 August 2017.
Pick up place: Ninh Kieu 1 Hotel Lobby.

For your accompanied family members to join the tour, please buy tickets from the conference secretary on 31 July.

Furthermore, on 3 August, Can Tho University will provide a free bus for participants to visit other tourist attractions near Can Tho, such as Khmer Temple in Soc Trang, Wind Power Farm and Nhà Công tử Bạc Liêu in Bac Lieu.

Program Timetable

Time	Monday 31 July	Tuesday 1 August	Wednesday 2 August
08:30 – 10:00	Opening (9:00) VTPS Young Research Awards Dao Vong Duc (O.1) *(Chair: Nguyen Ai Viet)*	Excursion (7:00 - 11:00)	Poster Session 2 (*Chair: Hoang Anh Tuan*)
10:00 – 10:30	Coffee break		Coffee break
10:30 – 12:00	Do Quoc Tuan (I.1) Le Duc Ninh (O.2) Do Thi Huong (O.3) Tran Xuan Nhut (O.4) *(Chair: Hoang Ngoc Long)*		Huynh Thanh Duc (O.15) Do Ngoc Son (O.16) Vu Ngoc Tuoc (O.17) Tran Van Quang (O.18) *(Chair: Bach Thanh Cong)*
12:00 – 14:00	Lunch		
14:00 – 15:30	Nguyen The Toan (O.5) Trinh Xuan Hoang (O.6) Ngo Son Tung (O.7) Le Duy Manh (O.8) *(Chair: Vu Ngoc Tuoc)*	Nguyen Van Chuong (I.2) Nguyen Mai Chung (O.12) Vu Thanh Tra (O.13) Nguyen Thi Thuy Nhung (O.14) *(Chair: Le Van Hoang)*	Phan Thi Ngoc Loan (O.19) Nguyen Thi Bich Duyen (O.20) Hoang Van Hung (O.21) Tran Cong Phong (O.22) *(Chair: Nguyen Quang Bau)*
15:30 – 16:00	Coffee break	Coffee break	Coffee break
16:00 – 17:30	Phung Van Dong (O.9) Dao Thi Nhung (O.10) Dang Van Soa (O.11) *(Chair: Dao Vong Duc)*	Poster Session 1 *(Chair: Dang Van Soa)*	Nguyen Tu Niem (O.23) Le Van Vinh (O.24) Nguyen Truong Long (O.25) *(Chair: Trinh Xuan Hoang)*
from 18:00	Gala Dinner (18:00 - 20:30)		

VTPS Young Research Awards

On July 31, at the opening session of the conference will be an announcement and the delivery of the 2017 VTPS Young Research Awards to Dr. Nguyễn Văn Chương (Le Quy Don Technical University) and Dr. Đỗ Quốc Tuấn (University of Science, Vietnam National University, Hanoi).

Conference Program

Monday, 31 July 2017

08:00 - 09:00 Registration

Opening Session
Chair: Nguyen Ai Viet

09:00 - 09:15 Opening

09:15 - 09:30 VTPS's Young Research Awards

09:30 - 09:50 O.1 – Oral
Massive gauge vector bosons in g(x)-deformed gauge imariance theory
Dao Vong Duc (Institute of Physics, VAST)

09:50 - 10:00 Photo Session

10:00 - 10:30 Coffee Break

Oral Session 1: *Particle and high energy physics*
Chair: Hoang Ngoc Long

10:30 - 11:00 I.1 – Invited
On the validity of cosmic no-hair conjecture in an anisotropic inflationary model
Đỗ Quốc Tuấn (Faculty of Physics, Vietnam National University, Hanoi)

11:00 - 11:20 O.2 – Oral
Weak gauge boson pair production at the LHC
Le Duc Ninh (Institute For Interdisciplinary Research in Science and Education (IFIRSE))

11:20 - 11:40 O.3 – Oral
A flipped trinification model for the current issues
Do Thi Huong (Institute of Physics, VAST)

11:40 - 12:00 O.4 – Oral
Neutrino Statistics and Current Cosmological Tensions
Truong Xuan Nhut (Institute For Interdisciplinary Research in Science and Education (IFIRSE))

12:00 - 14:00 Lunch Break

Oral Session 2: *Soft matter, biological and interdisciplinary physics*
Chair: Vu Ngoc Tuoc

14:00 - 14:20 O.5 – Oral
Grand-canonical Monte-Carlo simulation of solutions of salt mixtures: theory and implementation
Nguyen The Toan (Faculty of Physics, VNU University of Science, Vietnam National University)

14:20 - 14:40 O.6 – Oral
Folding of thick ribbons in a bad solvent
Trịnh Xuân Hoàng (Institute of Physics, VAST)

14:40 - 15:00 O.7 – Oral
Replica Exchange Molecular Dynamics Study of the Truncated Amyloid Beta (11-40) Trimer in Solution
Ngo Son Tung (Ton Duc Thang University)

15:00 - 15:20 O.8 – Oral
Behavior of heart rate responds to switching frequency
Le Duy Manh (Institute of Physics, VAST)

15:30 - 16:00 Coffee Break

Oral Session 3: *Particle and high energy physics*
Chair: Dao Vong Duc

16:00 - 16:20 O.9 – Oral
Left-right asymmetry and dark matter
Phung Van Dong (Institute of Physics, Vietnam Academy of Science and Technology)

16:20 - 16:40 O.10 – Oral
Higgs boson masses and Higgs decay widths in the NMSSM
Dao Thi Nhung (Institute For Interdisciplinary Research in Science and Education (IFIRSE))

16:40 - 17:00 O.11 – Oral
Implication of the 3-3-1 model for the cosmological issues and neutrino masses.
Dang Van Soa (Hanoi Metropolitan University)

18:00 - 20:30 Gala Dinner

Tuesday, 1 August 2017

08:00 - 12:00 Excursion

12:00 - 14:00 Lunch Break

Oral Session 4: *Condensed matter physics*
Chair: Le Van Hoang

14:00 - 14:30 I.2 – Invited
Tuning the electronic properties and Schottky barrier in the Graphene/MoS_2 van der Waals heterointerface by interlayer coupling
Nguyen Van Chuong (Le Quy Don Technical University)

14:30 - 14:50 O.12 – Oral
Theoretical study of electronic and thermoelectric nanodevices based on strained graphene junctions
Nguyen Mai Chung (Viện Vật Lý & Trường Đại học Khoa Học và Công Nghệ Hà Nội)

14:50 - 15:10 O.13 – Oral
Electronic structures in Penta - Graphene
Vu Thanh Tra (CanTho University)

15:10 - 15:30 O.14 – Oral
Determining the local density of states of circular graphene quantum dots: A transfer matrix approach
Nguyen Thi Thuy Nhung (Institute of Physics, Vietnam Academy of Science and Technology)

15:30 - 16:00 Coffee Break

Poster Session 1
Chair: Dang Van Soa

16:00 - 17:30 P.1 – Poster
Resonance energy transfer applied to improve the X-ray excited luminescence of CdSeS quantum dots for radiation detection
Phan Van Cuong (Nha Trang University)

16:00 - 17:30 P.2 – Poster
Electronic phase diagram in the half-filled ionic Hubbard model with site-dependent interactions
Hoang Anh - Tuan (Institute of Physics - VAST)

16:00 - 17:30 P.3 – Poster
Relation between branching ratios of the decay $h \to \mu\tau$ in minimal and inverse seesaw models
Tran Dinh Tham (Trường ĐH Phạm Văn Đồng, Quảng Ngãi)

16:00 - 17:30 P.4 – Poster
Study on elastic deformation of substitution alloy AB with interstitial atom C and BCC structure under pressure
Hiền Đức Nguyễn (Sở GD&ĐT Gia Lai)

16:00 - 17:30 P.5 – Poster
Study on the melting of substitution alloy AB with interstitial atom C and

FCC structure under pressure
Đinh Quang Vinh (Hanoi National university of Education)

16:00 - 17:30 P.6 – Poster
Popov-Fedotov functional integral approach for Heisenberg antiferromagnetic model on a non-Bravais lattice
Pham Thi Thanh Nga (Thuyloi University)

16:00 - 17:30 P.7 – Poster
Dynamics of Atomic Force Microscope Cantilevers dependent on the coating thickness
Le Tri Dat (University of Science HCMC)

16:00 - 17:30 P.8 – Poster
Molecular dynamics simulations of the melting of germanene
Nguyễn Hoàng Giang (Comp. Phys. Lab, HoChiMinh City Univ. of Technology, Vietnam National University – HoChiMinh City)

16:00 - 17:30 P.9 – Poster
Symmetric and asymmetric harmonic potential representations of q-deformed harmonic oscillator
Ngô Gia Vịnh (Sở Lao động và TBXH Bắc Ninh)

16:00 - 17:30 P.10 – Poster
Plasmon modes in graphene-GaAs heterostructures
Nguyễn Văn Mện (An Giang University; University of Science Ho Chi Minh City)

16:00 - 17:30 P.11 – Poster
Applying the modified perturbation theory to high energy scattering in the quasi-potential approach
Nguyen Nhu Xuan (Học viện Kỹ thuật Quân sự)

16:00 - 17:30 P.12 – Poster
Mechaleon mechanism in modified gravity f(R) of polynomial – exponential form
Vo Van On (University of Thu Dau Mot)

16:00 - 17:30 P.13 – Poster
Computational study of hydrogen adsorption in MIL-88 series
Nguyen Thi Xuan Huynh (University of Technology, VNU-HCM and Quy Nhon University)

16:00 - 17:30 P.14 – Poster
Magnetic orders in spin - one Heisenberg antiferromagnets on interpolating linear chain - square – triangular lattice: exact constraint of single occupancy condition
Pham Thi Thanh Nga (Thuyloi University)

16:00 - 17:30 P.15 – Poster

Energy spectra of single-layer graphene quantum rings
Đinh Thị Diệu Linh (Institute of Physics, VAST)

16:00 - 17:30 P.16 – Poster
Thermodynamic property of interstitial alloy FeCrSi with vacancy and BCC structure: Dependence on temperature, concentration of substitution atoms, concentration of interstitial atoms and concentration of equilibrium vacancies
Lê Hồng Việt (Tran Quoc Tuan University)

16:00 - 17:30 P.17 – Poster
The dynamics and structure heterogeneity in network forming liquids
Nguyen Thi Thanh Ha (Hanoi University of Science and Technology)

16:00 - 17:30 P.18 – Poster
Calculation of the Ettingshausen coefficient in a Rectangular quantum wire with an infinite potential in the presence of an Electromagnetic wave by using a Quantum kinetic equation
Nguyen Quang Bau (Faculty of Physics, Hanoi University of Science, VNU)

16:00 - 17:30 P.19 – Poster
The structures of multi-period electro-weak phase transition in the 3-3-1-1 model
Hoàng Ngọc Long (Viện Vật Lý, VHLKHCNVN)

16:00 - 17:30 P.20 – Poster
Distributions of neutron produced from (p,n) reaction on liquid lead target using for the accelerator driven subcritical reactor
Tran Minh Tien (Thu Dau Mot University)

16:00 - 17:30 P.21 – Poster
Pressure-induced structural transition in supercooled liquid and amorphous silicene via molecular dynamics simulation
Nguyen Truong Long (Can Tho University)

16:00 - 17:30 P.22 – Poster
Electronic properties of superlattice structures of AlN/GaN based on armchair nanoribbons
Huynh Thi My Duyen (College of Natural Sciences, Can Tho University)

16:00 - 17:30 P.23 – Poster
Develop a new tool for grading exam based on the Carbo quantum similarity and IQ curve: Application to Vietnam national exams 2012-2016
Chu Thuy Anh (Institute of Physics, VAST)

16:00 - 17:30 P.24 – Poster
Coherent potential approximation study of the three component Falicov-Kimball model
Nguyễn Thị Hương (Đại học Thuỷ Lợi)

16:00 - 17:30 P.25 – Poster

Drude-jellium model for microwave conductivity of electrolyte solutions
Tran Thi Nhan (Hanoi University of Industry)

16:00 - 17:30 P.26 – Poster
Melting of Two-Dimensional Crystal with Square Lattice Structure
Le Nguyen Tue Minh (Ho Chi Minh City University of Technology)

16:00 - 17:30 P.27 – Poster
Effects of macromolecular crowding on the escape of nascent proteins from the ribosomal tunnel
Bui Phuong Thuy (Nam Dinh University of Technology Education)

16:00 - 17:30 P.28 – Poster
Improvement the quantum teleportation via pair coherent states
Truong Minh Duc (Hue University, College of Education)

16:00 - 17:30 P.29 – Poster
Investigating the Influence of Dynamic-Core Polarization on High-Order Harmonics of Linear Molecules
Le Thi Cam Tu (Ho Chi Minh City University of Science)

16:00 - 17:30 P.30 – Poster
Magneto-optical absorption and cyclotron-impurity resonance in silicene
Le Thi Thu Phuong (University of Education, Hue University)

16:00 - 17:30 P.31 – Poster
Anomalous Velocity by Berry Curvature Effect in Semiconductor GaAs Quantum Well
Ngô Thành Công (Ho Chi Minh City Institute of Physics)

16:00 - 17:30 P.32 – Poster
Molecular Dynamics Simulation of Melting of 2D Glassy Monatomic Systems
Duong Thi Nhu Tranh (HochiMinh City Univ. of Technology, Vietnam National University – Ho Chi Minh City)

16:00 - 17:30 P.33 – Poster
Investigation of magneto-phonon resonance in graphene monolayers
Bui Dinh Hoi (University of Education, Hue University)

16:00 - 17:30 P.34 – Poster
Interplay between disorder, magnetism and topology in topological insulators doped with magnetic impurities
Nguyen Hong Son (Trade Union University)

16:00 - 17:30 P.35 – Poster
In Silico Study of Bombyx Mori Fibroin Enhancement by Graphene
Tran Thi Thu Hanh (Hochiminh City University of Technology)

16:00 - 17:30 P.36 – Poster
Cosmic inflation in modified gravity f(R) of polynomial – exponential form

Vo Van On (University of Thu Dau Mot)

16:00 - 17:30 P.37 – Poster

Simulations properties dynamics in Al2O3.2SiO2

Mai Van Dung (Thu Dau Mot University)

16:00 - 17:30 P.38 – Poster

Adsorption of CO_2 in metal organic framework of MIL-88a by computational methods

Son Do (University of Technology, VNU-HCM)

16:00 - 17:30 P.39 – Poster

A Tsallis entropy–based thermodynamic description of ecological systems

Le Van Xuan (Hanoi College of Technology and Economics)

16:00 - 17:30 P.40 – Poster

A model for enhancement factor and selection ruler of Surface Enhanced Raman Scattering

Duong Ha (Graduate University of Science and Technology, Vietnam Academy of Science and Technology)

Wednesday, 2 August 2017

Poster Session 2
Chair: Hoang Anh Tuan

08:30 - 10:00 P.41 – Poster

Energy of exciton in monolayer semiconductor WS2 with taken into account of modified Yukawa screening potential

Hoang Do Ngoc Tram (HCMC University of Education)

08:30 - 10:00 P.42 – Poster

The photon-drag effect in cylindrical quantum wire with an infinite potential for the case of electrons–acoustic phonon scattering

Hoang Van Ngoc (Hanoi University of sciences)

08:30 - 10:00 P.43 – Poster

Using generalized Bogoliubov transformation to study the collective behaviors of social complex systems

Chu Thuy Anh (Institute of Physics, VAST)

08:30 - 10:00 P.44 – Poster

The DFT Study of the Hydrogen Electroadsorption on the Missing Row Pt(110)-(1×2) Surface.

Tran Thi Thu Hanh (Hochiminh City University of Technology)

08:30 - 10:00 P.45 – Poster

Investigation of hydrogen adsorption in M(bdc)(ted)$_0$.5 by computer simulation methods

Nguyen Thi Xuan Huynh (University of Technology, VNU-HCM and Quy Nhon University)

08:30 - 10:00 P.46 – Poster

Problem of transition between Gaussian-like and Boltzmann-like forms of envelope functions in atomic and condensed mater physics

Mẫn Văn Ngữ (Hung Yen Industrial College)

08:30 - 10:00 P.47 – Poster

In silico Studies of Solvated F19W Amyloid β (11-40) Trimer

Ngo Son Tung (Ton Duc Thang University)

08:30 - 10:00 P.48 – Poster

Pressure-induced structural transition in supercooled liquid and amorphous silicene via molecular dynamics simulation

Huynh Anh Huy (Can Tho University)

08:30 - 10:00 P.49 – Poster

One loop corrections to decay $h^0 \to l_a l_b$ in economical 3-3-1 model

Le Thu Thuy (Can Tho University)

08:30 - 10:00 P.50 – Poster

Plasmon modes in Dirac/Schrödinger hybrid electron systems including layer-thickness and exchange-correlation effects

Nguyễn Văn Mện (An Giang University; University of Science Ho Chi Minh City)

08:30 - 10:00 P.51 – Poster

The crystallization of liquid iron nanoparticles

Nguyen Thi Thao (Faculty of Physics, Hanoi National University of Education)

08:30 - 10:00 P.52 – Poster

Surface optical phonon-assisted cyclotron resonance in monolayer phosphorene on polar substrates via two photon absorption process

Huỳnh Vĩnh Phúc (Dong Thap University)

08:30 - 10:00 P.53 – Poster

Spinor Tachyon of Gravitational Origin

Dao Vong Duc (Institute of Physics, VAST)

08:30 - 10:00 P.54 – Poster

Some application of q-deformed energy spectrum inverse problem and observer entanglement model of composite bosons

Nguyen Anh Sang (Hanoi Pedagogical University No. 2)

08:30 - 10:00 P.55 – Poster

Effect of exact thermal pairing on nuclear level density of even-even nuclei

Le Thi Quynh Huong (University of Khanh Hoa)

08:30 - 10:00 P.56 – Poster

Cooling rate effect and size effect on formation of two-dimensional SiC from the liquid state

Truong Quoc Tuan (Dept. of Physics, Faculty of Natural Sci., Can Tho Univ.)

08:30 - 10:00 P.57 – Poster

Tuning Electronic Properties of Transition Metal Dichalcogenides Monolayer by Polymer Doping

Ong Kim Le (University of Technology, VNU-HCM, Ho Chi Minh City, Vietnam)

08:30 - 10:00 P.58 – Poster

Cyclotron resonance linewidth in quantum wells with different phonon models

Nguyen Dinh Hien (College of Education, Hue University)

08:30 - 10:00 P.59 – Poster

Polar charges effect on multisubband electron mobility and linear intersubband optical absorption in the semiparabolic quantum wells based on AlN/AlGaN/AlN

Pham Thi Bich Thao (Can Tho University)

08:30 - 10:00 P.60 – Poster

Study of Influence of the anharmonic effect on changing size and shape of the material with the cubic crystal structure by an analytic statistical moment method.

Cao Huy Phuong (Hung vuong university)

08:30 - 10:00 P.61 – Poster

The electronic transport properties of the zigzag graphene nanoribbons

Nguyen Thanh Tien (Can Tho University)

08:30 - 10:00 P.62 – Poster

High-order harmonic generation from excited hydrogen molecular ion

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

08:30 - 10:00 P.63 – Poster

Dependence of Short-Channel Effects on Semiconductor Bandgap in Tunnel Field-Effect Transistors

Nguyễn Đăng Chiến (University of Dalat)

08:30 - 10:00 P.64 – Poster

Computer simulation of phase separation in 2D binary Lennard-Jones system

Duong Thi Nhu Tranh (HochiMinh City Univ. of Technology, Vietnam National University – Ho Chi Minh City)

08:30 - 10:00 P.65 – Poster

Structural and electronic properties of amorphous TiO_2 nanoparticles

Ca Nguyễn Anh Khoa (CanTho University)

08:30 - 10:00 P.66 – Poster

Theoretical investigation of quantum beat of excitons in GaAs/AlGaAs quantum wells

Lê Thị Ngọc Bảo (Trường Đại học Sư Phạm Huế)

08:30 - 10:00 P.67 – Poster

An A4 model with two Higgs singlets

Lam Hoang Thai (Cantho University)

08:30 - 10:00 P.68 – Poster

An application of q-deformed statistical method to lattice vibrations

Hoàng Hạnh Phương (Trường THPT Nam Sách,Hải Dương)

08:30 - 10:00 P.69 – Poster

Linear and nonlinear optically detected electrophonon resonance in triangular quantum wells

Pham Tuan Vinh (Dong Thap University)

08:30 - 10:00 P.70 – Poster

Effect of strain on electronic structure and thermoelectric property of a Bi2Te3/Sb2Te3 compound

Tran Van Quang (Department of Physics, University of Transport and Communications)

08:30 - 10:00 P.71 – Poster

Excitonic condensation phase diagram in the extended Falicov-Kimball model with electron-phonon interaction

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

08:30 - 10:00 P.72 – Poster

Production and decay of Higgs in the Randall-Sundrum model at high energy colliders

Bui Thi Ha Giang (Hanoi National University of Education)

08:30 - 10:00 P.73 – Poster

Controlling Band Gap of MoS2 Monolayer by Applying Pressure

Ong Kim Le (University of Technology, VNU-HCM, Ho Chi Minh City, Vietnam)

08:30 - 10:00 P.74 – Poster

Computational predictions of the new Gallium nitride nanoporous structures

Le Thi Hong Lien (Ha Noi University of Technology and Science)

08:30 - 10:00 P.75 – Poster

Investigation of Dark Matter in the $SU(3)_C \otimes SU(2)_L \otimes SU(3)_R \otimes U(1)_X$ model

Le Duc Thien (Viện vật lý)

08:30 - 10:00 P.76 – Poster

Computational Analysis of Fish Behavior Responses in Chemical Stress Using

Permutation Entropy and Fractal Dimension
Quach Kha Quang (Dong Thap University)

08:30 - 10:00 P.77 – Poster
Study of Crystal-Amorphous Phase Transition and Morphologies of Metal Nanoparticle Fe under annealing
Pham Huu Kien (Thainguyen University of Education)

08:30 - 10:00 P.78 – Poster
A study of non–extensive background fluctuation effect on a moving particle
Le Van Xuan (Hanoi College of Technology and Economics)

08:30 - 10:00 P.79 – Poster
The size of the metal nanoparticle dependence of fluorescence resonance energy transfer
Nguyen Minh Hoa (Hue university of Medicine and Pharmacy)

08:30 - 10:00 P.80 – Poster
Simulation of diffusion barrier and osmotic diffusion for single component systems
Vu Ba Dung (Hanoi University of Minging and Geology)

10:00 - 10:30 Coffee Break

Oral Session 5: *Condensed matter physics*
Chair: Bach Thanh Cong

10:30 - 10:50 O.15 – Oral
One-color photocurrents in noncentrosymmetric semiconductor quantum wells
Huynh Thanh Duc (Ho Chi Minh City Institute of Physics, VAST)

10:50 - 11:10 O.16 – Oral
Exploring Hydrogen Gas Adsorption in Co-MIL-88A by Computational Methods
Son Do (University of Technology, VNU-HCM)

11:10 - 11:30 O.17 – Oral
Theoretical prediction of the new ZnO nanoporous crystalline structures
Vu Ngoc Tuoc (Hanoi Univ. of Science and Technology)

11:30 - 11:50 O.18 – Oral
Electric-field modification of magnetism in a free-standing palladium ultrathin film
Tran Van Quang (Department of Physics, University of Transport and Communications)

12:00 - 14:00 Lunch Break

Oral Session 6: *Quantum optics and nanostructures*
Chair: Nguyen Quang Bau

14:00 - 14:20 O.19 – Oral

High-order harmonic generation from two-state hydrogen atom
Phan Thi Ngoc Loan (Ho Chi Minh City University of Education)

14:20 - 14:40 O.20 – Oral
Double Carbon-Doped Boron-Nitride Quantum Dots as Efficient Bifunctional Metal-Free Catalysts for Oxygen Reduction Reaction and Hydrogen Evolution Reaction: a Theoretical Study
Nguyen Thi Bich Duyen (Institute of Physics)

14:40 - 15:00 O.21 – Oral
Retrieval of target structure information from laser-induced photoelectrons and high-harmonic generation by few-cycle bicircular laser field
Hoàng Văn Hưng (Ho Chi Minh City University of Pedagogy)

15:00 - 15:20 O.22 – Oral
Cyclotron resonance via two-photon process in doped semiconductor superlattices with different confined phonon models
Tran Cong Phong (The Vietnam Institute of Educational Sciences)

15:30 - 16:00 Coffee Break

Oral Session 7: *Condensed matter physics*
Chair: Trinh Xuan Hoang

16:00 - 16:20 O.23 – Oral
Order-disorder phase transition in ultrathin ferroelectric perovskite films
Nguyễn Từ Niệm (VNU University of Science)

16:20 - 16:40 O.24 – Oral
Molecular dynamics simulations of pressure-induced structural changes in SiO2(1-x)Li2O(x) glasses
Le Van Vinh (Hanoi University of Science and Technology)

16:40 - 17:00 O.25 – Oral
Molecular dynamics study of crystallization of supercooled liquid and amorphous silicene
Nguyen Truong Long (Can Tho University)

17:00 - 17:30 Closing

Conference Abstracts

I.1 – Invited, NCTP-42

On the validity of cosmic no-hair conjecture in an anisotropic inflationary model

Tuan Q. Do

Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam

We will present main results of our recent investigations on the validity of cosmic no-hair conjecture proposed by Hawking and his colleagues long time ago in the framework of anisotropic inflationary model proposed by Kanno, Soda, and Watanabe. As a result, we will show that the cosmic no-hair conjecture seems to be generally violated in the Kanno-Soda-Watanabe model for both canonical and non-canonical scalar fields due to the existence of a non-trivial coupling term between scalar and electromagnetic fields. However, we will also prove that the validity of the cosmic no-hair conjecture will be ensured once an unusual scalar field called the phantom field, whose kinetic energy term is negative definite, is introduced into the Kanno-Soda-Watanabe model.

Presenter: Đỗ Quốc Tuấn

I.2 – Invited, NCTP-42

Tuning the electronic properties and Schottky barrier in the Graphene/MoS_2 van der Waals heterointerface by interlayer coupling

Chuong Van Nguyen (1), Nguyen Ngoc Hieu (2) Nguyen Van Hieu (3), Le Thi Phuong Thao (3), Le Thi Ngoc Tu (4)

(1) Le Quy Don Technical University; (2) Duy Tan University; (3) The University of Da Nang; (4) Dong Thap University

In the present work, the effect of interlayer coupling on structural and electronic properties of graphene/molybdenum disulfide (G/MoS_2) heterointerface is studied using density functional theory calculations. Our calculations show that weak van der Waals interactions between graphene and monolayer MoS2 are dominated at the interlayer distance of 3.34 Å and the binding energy per C atom of −25.1 meV. A narrow band gap of 3.6 meV has opened in G/MoS_2 heterointerface, and it can be modulated by the interlayer distance. Furthermore, the Schottky barrier and Schottky contact types in the G/MoS2 heterointerface can be controlled by the interlayer coupling. At the equilibrium state (d = 3:34 Å), the intrinsic electronic structure of G/MoS_2 heterointerface is well preserved and forms an n-type Schottky barrier of 0.49 eV. When the interlayer coupling decreases, the transition from n-type to p-type Schottky contact is occurred at d = 2:74 Å. Our studies may prove to promote the application of ultrathin G/MoS_2 heteroin-

terface in the next-generation nanoelectronic and photonic devices such as van-der-Waals-based field effect transistor.

Presenter: Nguyen Van Chuong

O.1 – Oral, NCTP-42

Massive gauge vector bosons in g(x)-deformed gauge imariance theory

Dao Vong Duc (1), Nguyen Mong Giao (2), and Tran Thanh Dung (3)

(1) Institute of Physics, VAST, Hanoi, Vietnam; (2) Center for Nuclear Research Ho Chi Minh Cit; (3) Thu Dau Mot University

In our recent works [1] a mechanism for mass creation in space-time with extra dimensions has been proposed and especially treated in more detail for vector bosons. Here we propose an alternative approach which gives the possibility for gauge vector bosons to acquire mass independently of Higgs mechanism. It is based on a modified gauge principle referred to as g(x)-deformed gauge imariance [2]. It also allows the possibility for the gauge coupling constants to be variable in space-time.

[1] D V Duc and N M Giao, J. of Moderm Phys. Vol 4, P 991 (2013); D V Duc et al., Intern. J. of Theor. Phys. Vol 54, P1071(2015); D V Duc and N M Giao, Intern. J. of Theor. Phys. Vol 55, P 959 (2016); [2] D V Duc et al., Vol 8, N1 (2017)

Presenter: Dao Vong Duc

O.2 – Oral, NCTP-42

Weak gauge boson pair production at the LHC

Le Duc Ninh

Institute For Interdisciplinary Research in Science and Education (IFIRSE)

Weak gauge boson pair production is an important process at the LHC because it probes the non-Abelian structure of electroweak interactions and it is a background process for many new physics searches. In this talk, after a review of the status of diboson production at the LHC, we will focus on the case of WZ production taking into account the effects of next-to-leading order electroweak corrections. We will also discuss polarization observables related to W and Z bosons.

Presenter: Le Duc Ninh

O.3 – Oral, NCTP-42

A flipped trinification model for the current issues

D. T. Huong (1), P. V. Dong (1), Jose W.F. Valle (2), and C.A. Vaquera-Araujo (2)

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We consider a flipped trinification model, which upgrades the theoretical and phenomenological aspects of the minimal left-right symmetric model. The model can explain small neutrino masses via a see-saw mechanism and naturally provide a dark matter candidate. The gauge coupling

unification and flavor physics at the LHC are briefly mentioned.

Presenter: Do Thi Huong

O.4 – Oral, NCTP-42

Neutrino Statistics and Current Cosmological Tensions

Truong Xuan Nhut (1,2), Marco Laveder (3), Stefano Gariazzo (4)

(1) Institute For Interdisciplinary Research in Science and Education (IFIRSE); (2) University of Rome 'Tor Vergata'; (3) University of Padova; (4) University of Valencia

Recent results from observations of the Cosmic Microwave Background (CMB) exhibit tensions with those obtained from astrophysical observations in the local Universe. In particular, CMB data from the Planck mission appears to prefer a significantly lower value of the current expansion rate (H0) than the one obtained from type Ia Supernovae Surveys (i.e. Riess et al. 2016). On the other hand, the Planck CMB predicts a higher value of the present-day amplitude of matter fluctuations, parametrized by the parameter sigma_8, with respect to the value derived from the Planck Sunyaev-Zeldovich Clusters observations. We seek for solution for the above tensions by provoking non-standard features from the neutrino sector. In our phenomenological study, which is motivated by previous works from particle physics side (Dolgov & Smirnov 2005, Dolgov et al. 2005), we consider a Lambda-CDM model in which neutrinos obey a mixed-statistics instead of the Fermi-Dirac distribution. In this talk, I will present our preliminary results, for the first time, on the power of current cosmological data, i.e. CMB, BAO, in constraining the neutrino statistics as well as its potential in solving the aforementioned tensions.

Presenter: Truong Xuan Nhut

O.5 – Oral, NCTP-42

Grand-canonical Monte-Carlo simulation of solutions of salt mixtures: theory and implementation

Duc Viet Nguyen, Toan T Nguyen

Faculty of Physics, VNU University of Science

In this work, we presented our investigation of the effect of ion sizes on the fugacities of salts and osmotic pressure of solution using the Grand-canonical Monte-Carlo (GCMC) simulation method. The GCMC method was presented in the preprint: arxiv.org/1705.08840v1. We study solution of 1:1, 2:1 and 2:2 salts or their mixtures at different concentrations using the primitive ion model. The osmotic pressures of the electrolyte solutions are calculated and shown to depend linearly on the salt concentrations within the concentration range simulated. Our work can explain some quantitative differences observed in experiments of the MgCl salt mixture and MgSO4 salt mixture.

Presenter: Nguyen The Toan

O.6 – Oral, NCTP-42

Folding of thick ribbons in a bad solvent

Thanh-Son Nguyen (1,2), Jayanth R. Banavar (3), Amos Maritan (4), and Trinh Xuan Hoang (1)

(1) Institute of Physics, Vietnam Academy of Science and Technology, Hanoi, Vietnam; (2) Liquid Crystal Institute, Kent State University, Kent, Ohio, USA; (3) University of Maryland, College Park, MD, USA; (4) University of Padova, Padova, Italy

Ribbons are intermediate between membranes/surfaces and polymers. They are important class of objects found in everyday life, in biology and nanotechnology. In this work, we study the folding of a thick and stiff ribbon in a poor solvent by using both exact arguments and Monte Carlo simulations. We find a rich phase diagram which reflects the dual characters of a ribbon with analogues to both polymers and membranes. The emergent conformations in this phase diagram include rolled (or Archimedian spiral), curled, twisted and globular conformations. The rolled and the curled conformations are akin to those of a membrane like a rolled carpet, whereas the globular conformation is similar to a compact polymer. Interestingly, both the ribbon thickness and the solvent molecule size are shown to moderate these dual characters. As an application, we show how our simple model of hydrophobic thick ribbon can be tailored to explain the formation of the celebrated DNA double helix structure.

Presenter: Trịnh Xuân Hoàng

O.7 – Oral, NCTP-42

Replica Exchange Molecular Dynamics Study of the Truncated Amyloid Beta (11-40) Trimer in Solution

Son Tung Ngo (1,2,), Huynh Minh Hung (3), Duc Toan Truong (4) and Minh Tho Nguyen (1,2,3)*

(1) Computational Chemistry Research Group, Ton Duc Thang University, Ho Chi Minh City, Vietnam; (2) Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam; (3) Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium; (4) Department of Theoretical Physics, Ho Chi Minh City University of Science, Ho Chi Minh City, Vietnam

Amyloid beta (Aβ) oligomers are neurotoxic compounds that destroy the brain of Alzheimer's disease patients. Recent studies indicated that the trimer is one of the most cytotoxic forms of low-weight Aβ oligomers. As there was limited information about the structure of Aβ trimer, either by experiment or computation, we determined in this work the structure of the 3Aβ11-40 oligomer for the first time using the temperature replica exchange molecular dynamics simulations with the appearance of explicit solvent. More than 20.0 μs of MD simulations were performed. The probability of the β-content and random coil structure of the solvated trimer amounts to 42 $\pm$ 6 and 49 $\pm$ 7 % that are in good agreement with experiments. Intermolecular interactions in central hydrophobic cores play a key role in stabilizing the oligomer. Intermolecular polar contacts between D23 and residues 24-29 replace the salt bridge D23-K28 to secure the loop region. The hydrophilic region of N-terminal is maintained by the intermolecular polar crossing contacts H13A-Q15B and H13B-Q15C. The difference in free energies of binding between the constituting monomers to the others is amounts to -36 $\pm$ 8 kcal/mol. The collision cross section of the representative structures of the trimer was computed to be 1330 $\pm$ 47 Å^2, that is in good agreement with previous experiments.

Presenter: Ngo Son Tung

O.8 – Oral, NCTP-42

Behavior of heart rate responds to switching frequency

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

(1) Institute of Physics, Vietnam Academy of Science and Technology, Hanoi, Vietnam; (2) Department of Physics and Graduate Institute of Physics, National Central University, Taoyuan, Taiwan; (3) Institute of Physics, Academia Sinica, Taipei, Taiwan

Recent pacing experiments with hearts of rat have discovered that the contractile response of the hearts can have an unexpected slow non-monotonic response. This later observation have not been reported and cannot be explained by the existing excitation-contraction (EC) coupling model. An improvement of discrete map model of the EC coupling is developed to understand these experimental findings. It is found that the biphasic response and the slow time scale can be reproduced when the model is integrated with the role of a very important enzyme, namely CaMKII – a protein complex that is well known to play an important role in Calcium homeostasis of the cardiac cells. Our improved model gives quite good agreement with the experimental data of heart rate in responding to switching frequency.

Presenter: Le Duy Manh

O.9 – Oral, NCTP-42

Left-right asymmetry and dark matter

P. V. Dong (1), D. T. Huong (1), T. D. Tham (2), N. C. Thao (3), and N. T. Nhuan (3)

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We propose a gauge theory, called left-right asymmetry, which automatically provides dark matter from its first principles. R-parity that stabilizes dark matter originates as a residual gauge symmetry and is related to the electric charges. The dark and normal matters are unified in the gauge multiplets. The theory recognizes the TeV WIMP scenarios, which satisfy the relic density and experimental searches.

Presenter: Phung Van Dong

O.10 – Oral, NCTP-42

Higgs boson masses and Higgs decay widths in the NMSSM

Dao Thi Nhung

Institute For Interdisciplinary Research in Science and Education (IFIRSE)

The Next-to-Minimal Supersymmetric Standard Model (NMSSM) is the supersymmetric extension of the Standard Model with an extra complex singlet field. The model has received an intensive study thanks to its rich phenomenology. In this talk I will discuss about the higher order correction to the Higgs boson masses and their decay width in NMSSM. The inclusion of higher order effects is extremely important in the interpreting correctly Higgs data at the LHC.

Presenter: Dao Thi Nhung

O.11 – Oral, NCTP-42

Implication of the 3-3-1 model for the cosmological issues and neutrino masses

D. V. Soa (1), P. V. Dong (2), D. T. Huong(2) and L. D. Thien (2)

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

We consider the 3-3-1 model at a large scale which addresses the neutrino masses, superheavy dark matter, and inflation. Phenomenology of the model is presented in details.

Presenter: Dang Van Soa

O.12 – Oral, NCTP-42

Theoretical study of electronic and thermoelectric nanodevices based on strained graphene junctions

M. Chung Nguyen (1,2,3), V. Hung Nguyen (1,2), H. Viet Nguyen (1) and P. Dollfus (2)

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Graphene, due to its outstanding physical properties, is expected to be able to replace or, at least, complement traditional semiconductors in device technology [1]. However, applications of graphene in electronic devices are still questionable because of its gapless character. In particular, regarding electronic applications, the absence of energy bandgap in the electronic band structure makes it difficult to switch off the current in graphene devices like transistors [2]. For thermoelectric properties, the gapless character is also a strong drawback since it prevents the separation of the opposite contributions of electrons and holes to the Seebeck coefficient [3]. Thus, opening a sizable bandgap in graphene is required to overcome the disadvantages of graphene and to fully benefit from its excellent conduction properties. Although many nanostructuring techniques can be used to open such a bandgap in graphene, e.g., graphene nanoribbons, graphene bilayer with a perpendicular electric field, graphene nanomesh lattices, channels based on vertical stack of graphene layers , mixed graphene/hexagonal boron nitride structures, nitrogen doped graphene, etc, each of these methods has its own fabrication issues and/or need to be further confirmed by experiments.

In this work, we present our theoretical studies focusing on strain engineering, which offers a wide range of opportunities for modulating the electronic properties of graphene nanostructures. We show that with a strain of only a few percent, the strain-induced shift of the Dirac point in k-space may be enough to open a sizable conduction gap (500 meV or more) in graphene heterojunctions made of unstrained/strained junctions [4]. The effect can be exploited to improve the behavior and performance of several types of devices. We show that, with a strain of only 5%, it is possible to switch off transistors efficiently, with the ON/OFF current ratio of several order of magnitude larger than that of pristine graphene transistors which is not exceeding 10 [5]. By combining strain and doping engineering Seebeck coefficient can reach values higher than 1.4 mV/K, which is 17 times higher than in gapless pristine graphene [6]. This makes graphene an excellent candidate for thermoelectric material as well. Finally, we will show that very strong negative differential conductance (NDC) effects with peak-to-valley ratios of a few hundred at room temperature can be achieved by using appropriate strain engineering in graphene diodes made of either single gate-induced strained barrier or a p-n junction [7].

[1] A. C. Ferrari et al., Nanoscale 7, 4598 (2015). [2] Ha et al, Electron Device Lett. IEEE 34, 559 (2013). [3] Zuev et al, Phys. Rev. Lett. 102, 096807 (2009). [4] M. C. Nguyen et al., Semicond. Sci. Technol. 29,115024(2014). [5] V. H. Nguyen et al., Nanotechnology 25, 165201 (2014). [6]

M. C. Nguyen et al., Physica E 73, 207(2015). [7] M. C. Nguyen et al., J. Appl. Phys. 118, 234306(2015).

Presenter: Nguyen Mai Chung

O.13 – Oral, NCTP-42

Electronic structures in Penta - Graphene

Vu Thanh Tra (1), Thai Thanh Lap (2), Nguyen Thi Kim Quyen (2)

(1) Department of Physics, School of Education, Can Tho University, Can Tho, Vietnam; (2) School of Graduate, College of Natural Sciences, Can Tho University, Can Tho, Vietnam

Recently, Penta – Graphene is known as a new outstanding of carbon allotrope. This structure consists of sp2 - hybridized carbon atoms also sp3 - hybridized carbon atoms which makes its electronic properties more interesting than others. The electronic band structures of this new material have been studied using in this paper by indicating different parameters' contributions. Especially, this model is supplemented interaction between sp2 - hybridized carbon atoms and the nearest 2nd – neighbor atoms that leads these results to reliance and preciseness. Moreover, this study shows that, unlike Graphene, the onsite energy of sp2 - hybridized carbon atoms in this structure is not zero. Therefore, the significance of structure parameters in energy band is pointed out which have not discussed in other researches. Furthermore, for convincing investigation of the energy band, we continued to calculate the density of states and the transmission coefficient by using Green's function formalism. More importantly, we consider the effect of vertical electric fields on the electronic properties of Penta - Graphene with hoping to control the gap. These results are important to fully understand structure of Penta – Graphene and motivate to Penta – Graphene for applications in nano electronics.

Presenter: Vu Thanh Tra

O.14 – Oral, NCTP-42

Determining the local density of states of circular graphene quantum dots: A transfer matrix approach

H. Chau Nguyen (,1) Nhung T. T. Nguyen (2,3) and V. Lien Nguyen (2,4)*

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Graphene quantum dots (GQDs) are unlike conventional semiconductor quantum dots in that they can only trap charge carriers for short times in the so-called quasi-bound states, primarily due to the effect of Klein tunneling. This particular property of GQDs is associated with broad resonance peaks in their local density of states (LDOS). In this work, we propose a method based on the transfer matrix formalism to calculate the local density of states of any circular graphene quantum dot induced by an axially symmetric electrostatic potential on a continuous graphene sheet. Our calculations using a square potential for the graphene quantum dot studied in a recent scanning tunneling microscopy measurement [Gutierrez et al. Nat. Phys. 12, 1069 (2016)] show an excellent agreement between theory and experiment. We also find that resonance

widths extracted from our calculated LDOS are consistent with experimental values and match those obtained from the complex energy spectrum of the corresponding Dirac equations. Our method can be used to study the effect of potential shape. As an application, we have calculated the LDOS for a graphene quantum dot with a Lorentzian shape potential and suggest that this potential shape corresponds to that induced by the charged STM-tip in another reported experiment [Schneider & Brouwer, PRB 89, 205437 (2014)].

Presenter: Nguyen Thi Thuy Nhung

O.15 – Oral, NCTP-42

One-color photocurrents in noncentrosymmetric semiconductor quantum wells

Huynh Thanh Duc

Ho Chi Minh City Institute of Physics, VAST

We present an unified microscopic approach that is capable of describing fully dynamically all three kinds of one-color photocurrents in noncentrosymmetric semiconductor quantum wells, i.e., injection, shift, and rectification currents. Our approach has been applied to analyze photocurrents generated by circularly and linearly polarized laser pulses in [110]-oriented GaAs/AlGaAs quantum wells. Calculation results are compared to experiments and good agreement is obtained.

Presenter: Huynh Thanh Duc

O.16 – Oral, NCTP-42

Exploring Hydrogen Gas Adsorption in Co-MIL-88A by Computational Methods

Do Ngoc Son (1,), Nguyen Thi Xuan Huynh (1,2), O My Na (1)*

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Unsaturated metal centers in metal-organic framework MIL-88A are able to significantly enhance the amount of gas adsorbed at ambient temperatures and low pressures. This material has been investigated for various applications; however, it has not yet been tested for hydrogen storage. In this research, we examined the interaction of hydrogen gas with Co-MIL-88A by using the van der Waals dispersion-corrected density functional theory calculations. The H2 molecule was found to adsorb most favorably at the hollow site of the metal trimers in Co-MIL-88A because of the maximum overlap between the bonding state of the hydrogen molecule and the total density of state of the Co-MIL-88A. In addition, the hydrogen adsorption isotherms were also assessed by grand canonical Monte Carlo simulations. The results showed that Co-MIL-88A is one of the most effective hydrogen gas storage materials.

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Presenter: Son Do

O.17 – Oral, NCTP-42

Theoretical prediction of the new ZnO nanoporous crystalline structures

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Nanoporous framework materials capture a great deal of research attention because of their advantages for a wide range of technology applications in the environment, sensors, shape-selective and bio-catalysis, to name just a few. Within this active research area, computational prediction and theoretical study of these materials are crucial important. We have designed a large family of ZnO nanoporous crystalline structures employing the density functional theory based methods. Our modeling scheme is based on the two approach, "bottom up" and "top down" designs, owing to the advanced nanofabrication techniques. Depend on their secondary building blocks, e.g. ZnO magic cluster cages, nanowire, nanosheet, quantum dot, our modeling crystalline can classified as cage-like hollow, hollow channel, hollow quantum dot nanoporous. For the structural stability, our calculations show that these nanoporous structures could survive in periodic systems without structural collapse, which leads to nanoporous low-density phases of ZnO. Their electronic and thermodynamical properties of the structures, e.g., band structure, free energy and simulated XRD patterns are calculated and discussed in the connection with hollow properties, i.e. shape, size and wall thickness and in the relation with their symmetry. Our results show the convergence of nonlinear depends of bulk modulus on hollow's thicknesses of about of larger than three layers regarding to hollow-to-bulk density ratio and the common rule for the dependences on porosity for different type of hollow topology. We also found that these ZnO hollow phases, if synthesized, would preserve the valuable properties of the ZnO materials, such as wide bandgap semiconducting, piezoelectric and optically transparent, while, at the same time, would possess novel properties as of gap engineering possibility. Keywords: ZnO nanoporous, structure prediction, density functional theory

Presenter: Vu Ngoc Tuoc

O.18 – Oral, NCTP-42

Electric-field modification of magnetism in a free-standing palladium ultra-thin film

Tran Van Quang

Department of Physics, University of Transport and Communications, Hanoi, Vietnam

Recently, several magnetic properties have been found to be tunable with an applied electric field, which enabled the electrically assisted magnetic recording. In this work, we performed first-principles calculation to demonstrate that the electric field produces a surface magnetoelectric effect on a free-standing palladium ultra-thin film. We consider a bilayer strained Pd film in vacuum within an external electric field. The magnetic moment of Pd is found to be unchanged under an applied electric field below a critical value, E_c whereas the change follows a square-root variation with the electric field above E_c. This is originating from induced spin density of d-states. Under the electric field, the Fermi energy is likely to be shifted to increase majority spin density whereas it reduces the minority one. The major change is found in the occupancies of $d_{(x^2-y^2)}$, d_{xy} and d_{xz}. This feature is responsible for the magnetoelectric coupling.

Presenter: Tran Van Quang

O.19 – Oral, NCTP-42

High-order harmonic generation from two-state hydrogen atom

Ngoc-Loan T. Phan, Thanh-Tuynh T. Nguyen, Van-Hung Hoang

Department of Physics, Ho Chi Minh City University of Pedagogy

High-order harmonic generation (HHG) emitted from hydrogen atom with coherent superposition of the ground and first excited states, exposed to an intense ultra-short laser pulse is systematically studied in this work. First, we discuss in detail how the contribution of initial population of excited state affect on the intensity of HHG spectra, and show that HHG conversion efficiency is extremely sensitive to the existence of the excited state. Second, we demonstrate the appearance of the multi-cutoff in HHG spectra when intense laser with long wavelength is used. Moreover, we claim that this multi-cutoff effect occur due to the depletion phenomenon and a clear explanation is also given.

Presenter: Phan Thi Ngoc Loan

O.20 – Oral, NCTP-42

Double Carbon-Doped Boron-Nitride Quantum Dots as Efficient Bifunctional Metal-Free Catalysts for Oxygen Reduction Reaction and Hydrogen Evolution Reaction: a Theoretical Study

Nguyen Thi Bich Duyen, Tran Nguyen Lan*

Ho Chi Minh City Institute of Physics, VAST, Ho Chi Minh City, Vietnam

Fuel cells have attracted significant attention due to their high efficiency and low pollution. While platinum has been shown to be an effective material for catalyzing the oxygen reduction and hydrogen evolution reaction (ORR and HER) in fuel cells, its scarcity and cost has rendered it impractical for large-scale applications. Therefore, many alternative catalytic materials are being actively researched such as transition metal compounds, metal-free catalyst... Among of them, metal-free ORR/HER bifunctional catalyst have been also extensively considered in recent years. However, to the best of my knowledge, no metal-free ORR/HER or ORR/OER (oxygen evolution reaction) bifunctional catalyst using Boron-Nitride (BN) materials has been reported. In this study, using density functional theory, it is the first time to show that double C-doped Boron-Nitride quantum dots (BNQDs) can be used as ORR/HER bifunctional catalyst. Hereafter, we consider the cases of two C atoms substituting different positions such as two N and B atoms namely 2CN-BNQDs and 2CB-BNQDs, respectively. Firstly, we found that both of them can happen via two main pathways: dissociative and associative pathway in ORR. Obviously, the former one is more energetically favorable than the later one, which can be attributed to double active sites in double C-doped BNQDs.

Presenter: Nguyen Thi Bich Duyen

O.21 – Oral, NCTP-42

Retrieval of target structure information from laser-induced photoelectrons and high-harmonic generation by few-cycle bicircular laser field

Van-Hung Hoang (1, 2), Van-Hoang Le (1), Anh-Thu Le (2)

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Photoelectron momentum and high-harmonic generation for atoms in few-cycle bicircular laser pulses are obtained by solving time-dependent Schrodinger equation numerically. We show that

high-energy photoelectron momentum spectra can be used to extract accurate elastic scattering differential cross sections of the target ion with free electrons. We also show that high harmonic generation can be understood within the quantitative rescattering theory. Our results are in a good agreement with recent experiments from Baykusheva et al (ETH). We further show that HHG yield and phase are not sensitive with respect to macroscopic propagation condition. This offers a potentially powerful tool for more accurate HHG spectroscopy in the future.

Presenter: Hoàng Văn Hưng

O.22 – Oral, NCTP-42

Cyclotron resonance via two-photon process in doped semiconductor superlattices with different confined phonon models

Vo Thanh Lam (1), Le Trung Dung (2), Nguyen Dinh Hien (2), and Tran Cong Phong (3)

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Cyclotron resonance via two photon absorption processes in doped semiconductor superlattices (DSSL) is theoretically studied with different confined phonon models (the Fuchs-Kliewer slab, Ridley's guided, and Huang-Zhu models). The full-widths at half-maximum (FWHM) for the intra- and inter-subband transitions are defined as functions of the magnetic field, temperature, and ratio of confinement frequencies. The obtained results help us to explain why phonons can effect on the FWHM while the energy is not contained in the CR condition. The results also show that cyclotron resonance FWHM in the cases of confined phonons varies faster and has a larger value than it does for the bulk phonon case and in all range of the confinement frequency, the phonon confinement becomes more important and should be taken into account in studying the FWHM although it is for two-photon process. Besides, the cyclotron resonance FWHM is found largest for Huang-Zhu model among the three confined phonons models, while it is smallest for guided mode model case

Presenter: Tran Cong Phong

O.23 – Oral, NCTP-42

Order-disorder phase transition in ultrathin ferroelectric perovskite films

Nguyen Tu Niem, Bach Thanh Cong

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The order-disorder phase transition in ferroelectric films down to nanoscale thickness is usually explained within the framework of the famous Landau-Ginzburg-Devonshire theory. But for ultrathin films consisting from few atomic layers, the problem is still opened. In this report, the thermodynamic theory for the ultrathin ferroelectric perovskite films (UFPF) is developed using the Ising model in transverse field and mean field approximation. It is shown that, the polarization, entropy, specific heat phase transition temperature of the UFPF are strongly affected by the thickness and transverse field. Dependence of the critical thickness (thickness below that the ferroelectric order is destroyed) on the thickness and transversal field is also discussed and calculated for several UFPF.

Presenter: Nguyễn Từ Niệm

O.24 – Oral, NCTP-42

Molecular dynamics simulations of pressure-induced structural changes in SiO2(1-x)Li2O(x) glasses

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Molecular dynamics (MD) simulations of [SiO2](x-1)[Li2O](x) glasses have been carried out to investigate the pressure-induced structural transformation. The local atomic structure was analyzed through the pair radial distribution functions, bond angle distributions, coordination number, void statistics and common neighbor analysis. We found that the distribution of Li is fairly uniform in all samples. With increasing pressure, O atoms are more ordered than Si and Li atoms and to form hcp cluster. The change of local atomic structure upon compression has been also presented. Keywords: Molecular dynamics, SiO2, Li2O, glass, compression.

Presenter: Le Van Vinh

O.25 – Oral, NCTP-42

Molecular dynamics study of crystallization of supercooled liquid and amorphous silicene

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Crystalline-Amorphous transition under isothermal condition of supercooled liquid and amorphous silicene (a-silicene) models has been studied via molecular dynamics (MD) simulation with Stillinger-Weber (SW) interaction potential. Supercooled liquid and a-silicene models containing 10000 atoms are obtained by rapid cooling process from the melts. At each given temperature below and above Tg, models are annealed for 10 nanoseconds in order to investigate aging effect on two-dimensional structural arrangement of disordered Si-atoms. Time dependence thermodynamic and structural quantities are analyzed including total energy, radial distribution function (RDF), coordination number, interatomic distance, ring and bond-angle distribution. Insights of "natural" re-formation process of disorder state models via 2D visualization of atomic configurations is presented. Our calculation shows that 2D-crystallization of supercooled liquid and a-silicene exhibits a first-order behavior, however, the aging effect takes place almost immediately after relaxation. Atomic mechanism of crystallization is studied in details during annealing process and we clarify novel scenario of crystallization. Homogeneous natural quenched-in nucleated atoms have a tendency to aggregate into larger clusters in 2D Si supercooled liquid sheet. In contrast, the phase transition of a-silicene shows a partial crystallization and crystal clusters are found to be heterogeneously grown in models below Tg. Crystalline formation below Tg results in a quasi-equilibrium state with a large amount of defects after a long relaxation time. In all crystallized models, we found that the existence of low-numbered ring chains which may play an important role in controlling the crystal structure in practice.

Acknowledgements: This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under Grant 103.02-2016.88.

Presenter: Nguyen Truong Long

P.1 – Poster, NCTP-42

Resonance energy transfer applied to improve the X-ray excited luminescence of CdSeS quantum dots for radiation detection

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The sensitivity, response time, and energy resolution of scintillators are very important properties for radiation detection. To meet these requirements, quantum dot (QD) scintillators such as CdSe, CdSeS, and CdTe must have very high quantum efficiencies, as a consequence of quantum size confinement, of up to 98% and short luminescence lifetimes in the nanosecond range. In general, semiconductor QDs could be promising for radiation detection because of their short lifetimes and high sensitivities. However, the disadvantage is that the stopping power of most II–VI QDs is low and their scintillation luminescence is very weak.

In this paper, we report a method, which can be used to overcome the above limits. In detail, the X-ray excited luminescence (XEL) of CdSeS QDs was enhanced considerably in the presence of LaF3:Ce nanoparticles (NPs). In step one, the LaF3:Ce NPs were synthesized in water solution; in step two, the CdSeS QDs were prepared; in step three, the LaF3:Ce NPs were combined with the CdSeS QDs to form a LaF3:Ce/CdSeS nanocomposite. The average diameter of nanocomposite is about 12 nm.

The products were characterized and analyzed using an X-ray diffractometer (Rigaku D/Max2500, Cu-Kα radiation, λ=1.54178 Å) and field-emission transmission electron microscope (FE-TEM – Titan G2 ChemiSTEM Cs Probe from FEI Co.). The photoluminescence (PL) of the nanocomposites at room temperature were measured under excitation by an iHR320 imaging spectrometer (Horiba Jobin Yvon). The XEL of the LaF3:Ce/CdSeS nanocomposite at room temperature was measured using a QE65000 fiber optic spectrometer (Ocean Optics) under excitation by an X-ray tube with a W anode (DRGEM Co.).

The XEL of CdSeS QDs was negligible; however, the combination of LaF3:Ce NPs (high stopping power and sensitivity) with CdSeS QDs (high emission rate and emission tenability) can help the XEL of CdSeS QDs improve significantly, which can be ascribed to the efficient resonance energy transfer (RET) from LaF3:Ce NPs to the CdSeS QDs in the LaF3:Ce/CdSeS nanocomposite. This RET-based approach could be applied to functional nanomaterials used in radiation detectors.

Presenter: Phan Van Cuong

P.2 – Poster, NCTP-42

Electronic phase diagram in the half-filled ionic Hubbard model with site-dependent interactions

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A repulsive Hubbard model with spatially alternating interactions ($U_A \neq U_B$) and a staggered potential, which may be realized by cold atoms in optical lattices, is studied by means of the coherent potential approximation. The paramagnetic phase diagram for the half-filled model is

obtained. It is found that for the model with $U_A \neq U_B$ a metallic region considerably enlarges in comparison with that of the conventional ionic Hubbard model ($U_A = U_B$).

Presenter: Hoang Anh - Tuan

P.3 – Poster, NCTP-42

Relation between branching ratios of the decay $h \to \mu\tau$ in minimal and inverse seesaw models

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The branching ratios (Br) of lepton flavor violating decay of the standard-model-like Higgs bosson (LFVHD) $h \to \mu\tau$, predicted by the minimal (MSS) and inverse (ISS) seesaw models, are compared to explain why these models predict very different values of Brs. We will show that these Brs enhance with large and increasing heavy new neutrino mass scale m_{n_6}. The ratio between two branching ratios predicted by the ISS and MSS can be estimate by a simple factor $m^2_{n_6}\mu_X^{-2}$, where μ_X is the small neutrino mass term appearing in the ISS only.

Presenter: Tran Dinh Tham

P.4 – Poster, NCTP-42

Study on elastic deformation of substitution alloy AB with interstitial atom C and BCC structure under 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 E, the bulk modulus K, the rigidity modulus G and the elastic constants C11, C12, C44 for substitution alloy AB with interstitial atom C and BCC structure under pressure are derived from the statistical moment method. The elastic deformations of main metal A, substitution alloy AB and interstitial alloy AC are special cases of elastic deformation for alloy ABC. The theoretical results are applied to alloy FeCrSi. The numerical results for alloy FeCrSi are compared with the numerical results for main metal Fe, substitution alloy FeCr, interstitial alloy FeSi and experiments.

Presenter: Hiền Đức Nguyễn

P.5 – Poster, NCTP-42

Study on the melting of substitution alloy AB with interstitial atom C and FCC structure under pressure

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(1) Hanoi National University of Education, 136 Xuan Thuy, Cau Giay, Hanoi; (2) University of Transport and Communications, 3 Cau Giay, Dong Da district, Hanoi

From the model of substitution alloy AB with interstitial atom C and FCC structure and the

condition of absolute stability for crystalline state we derive analytic expression for the temperature of absolute stability for crystalline state, the melting temperature and the equation of melting curve of this alloy by the way of applying the statistical moment method. The obtained results allow us to determine the melting temperature of alloy ABC ant zero pressure and under pressure. In limit cases, we obtain the melting theory of main metal A, substitution alloy AB and interstitial alloy AC with FCC structure. The theoretical results are numerically applied for alloys AuCuSi and AgCuSi. Keywords: interstitial and substitution alloy, absolute stability of crystalline state, statistical moment method.

Presenter: Đinh Quang Vinh

P.6 – Poster, NCTP-42

Popov-Fedotov functional integral approach for Heisenberg antiferromagnetic model on a non-Bravais lattice

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We use the Popov-Fedotov formalism for studying magnetic properties of the Heisenberg antiferromagnetic (HAF) model on a non-Bravais lattice. The spin operators are represented by auxiliary canonical fermions and the local constraint is exactly treated by introducing an imaginary chemical potential. Working on a local coordinate system we obtain a sublattice magnetization, free energy and other thermo-dynamical quantities in unique forms for different non-Bravais lattice structures in magnetically ordered phases taking into account fluctuations in one loop approximation. As an example we get the explicit expressions for the case of honeycomb lattice and compare them with the results of slave boson theory.

Presenter: Pham Thi Thanh Nga

P.7 – Poster, NCTP-42

Dynamics of Atomic Force Microscope Cantilevers dependent on the coating thickness

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We study the dynamics of an atomic force microscope cantilever under irradiation of laser. Thermally induced effects change the deflection and the resonance frequency of the cantilever. For input power less than 10 μW and a coating thickness with of 20-140 nm, these values can evaluate dynamics of cantilever. The temperature distribution along cantilever and the cantilever deflection is dependent on the coating thickness.

Presenter: Le Tri Dat

P.8 – Poster, NCTP-42

Molecular dynamics simulations of the melting of germanene

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By using molecular dynamics (MD) simulation, we compute the model containing 10000 Ge atoms interacted via the Stillinger-Weber potential. The model has the fixed length of the z direction which equals to the buckling length of 0.737Å with the elastic reflection behavior boundary. In this work, we show the phase transition picture of germanene buckling 2D membrane from the solid state to the liquid state at the atomic level. Radial distribution functions, coordination numbers, ring statistics, interatomic distances, bond-angle distributions are investigated in details. Besides, the formation of defects destroying the crystal state of germanene membrane is presented clearly. Our result shows that the phase-transition temperature of this material in the buckling 2D model is about 1670 K which is higher than the melting temperature of the bulk model of germanium (with K) due to confinement in the direction of the former. Atomic mechanism of melting of the buckling 2D germanene is discussed in details. Similar mechanism of melting for other buckling 2D analogs such as silicene can be suggested. This research is funded by Vietnam National University - Ho Chi Minh City (VNU-HCM) under grant number B2017-20- 02.

Presenter: Nguyễn Hoàng Giang

P.9 – Poster, NCTP-42

Symmetric and asymmetric harmonic potential representations of q-deformed harmonic oscillator

Ngo Gia Vinh (1), Man Van Ngu (2), Nguyen Tri Lan (3), Le Minh Thanh (4) ,Nguyen Thi Dung (5), Nguyen Khac Ngoc (2), Nguyen Ai Viet (3)

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The problem of q-deformed harmonic oscillator in asymmetric and symmetric potential representations is proposed. The connection between the statistical properties of systems and these representations of q-deformed harmonic oscillator is assumed and investigated. A possibility of direct and inverse ways to use these models is shown for some real physical problems.

Presenter: Ngô Gia Vịnh

P.10 – Poster, NCTP-42

Plasmon modes in graphene-GaAs heterostructures

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We investigate the plasmon dispersion relation and damping rate of collective excitations in a double-layer system consisting of bilayer graphene and GaAs quantum well, separated by a distance, at zero temperature with no interlayer tunneling. We use the random-phase-approximation dielectric function and take into account the nonhomogeneity of the dielectric background of the system. We show that the plasmon frequencies and damping rates depend considerably on interlayer correlation parameters, electron densities and dielectric constants of the contacting media.

Presenter: Nguyễn Văn Mện

P.11 – Poster, NCTP-42

Applying the modified perturbation theory to high energy scattering in the quasi-potential approach

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(1) Department of Theoretical Physics, Hanoi National University, Vietnam; (2) Department of Physics, Le Qui Don University, Hanoi, Vietnam

Asymptotic behavior of the scattering amplitude for two scalar particles at high energy and fixed momentum transfers is reconsidered in quantum field theory. In the framework of the quasi-potential approach and using the modified perturbation theory the leading eikonal scattering amplitude and its corrections are constructed. Also, the differential cross section is discussed. Several interaction potentials, Yukawa, Gauss and Newton are used to illustrate the problem.

Presenter: Nguyen Nhu Xuan

P.12 – Poster, NCTP-42

Mechaleon mechanism in modified gravity f(R) of polynomial – exponential form

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(1) Department of Physics, Faculty of Natural Sciences, University of Thu Dau Mot; (2) Faculty of natural Sciences, Can Tho University

In this paper, we firstly outline the Chameleon mechanism in the class of theory of modified gravity of f (R), and then apply it in the polynomial – exponential theory of f(R) to find the constraints from the solar system to the parameters α and β of this model. Calculated results show that the chameleon mechanism satisfies easily in the polynomial - exponential theory of f(R), the constraints on the beta and alpha parameters are as follows: $0 < \beta <$0.076; $0 < \alpha <$10-46.

Presenter: Vo Van On

P.13 – Poster, NCTP-42

Computational study of hydrogen adsorption in MIL-88 series

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Metal organic frameworks with open metal sites are promising candidates for gas capture and storage. MIL-88 series is highly stable in the humid environment, and hence it may be good for hydrogen storage based on the adsorption phenomenon. In this work, we are concerned with the hydrogen adsorption in MIL-88 series. Electronic structure properties of hydrogen adsorption were studied by using the van der Waals dispersion-corrected density functional theory. Simultaneously, the hydrogen uptake capacity in MIL-88s was evaluated by using the grand canonical Monte Carlo simulation. From the obtained results, we can clarify the concerns of the present work. Acknowledgement. This research was funded by the Vietnam National

Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2017.04.

Presenter: Nguyen Thi Xuan Huynh

P.14 – Poster, NCTP-42

Magnetic orders in spin - one Heisenberg antiferromagnets on interpolating linear chain - square - triangular lattice: exact constraint of single occupancy condition

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We study the spin - one antiferromagnetic Heisenberg model on a square lattice with nearest neighbor interaction J1 and a second neighbor interaction J2 along only one of the diagonals of the squares using the Popov-Fedotov representation of spin operators. In this approach the constraint of single particle site occupation is rigorously fulfilled by introducing an imaginary valued chemical potential. We consider a Neel antiferromagnetic phase and an incommensurate spiral phase in one loop approximation. The results are compared with the results obtained by the same formalism for the case of spin - one and by Holstein-Primakov representation for the case of spin half.

Presenter: Pham Thi Thanh Nga

P.15 – Poster, NCTP-42

Energy spectra of single-layer graphene quantum rings

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Quantum rings have been originally studied in the physics of metal/semiconductor nanostructures. The ring geometry results in a specific energy spectrum and allows to observe the most basic quantum phenomena such as the Aharonov-Bohm (AB) effect and the related persistent current (i.e. the equilibrium current driven by the magnetic field threading the ring). Graphene, a single layer of carbon atoms in a honeycomb lattice, shows unique electronic properties such as the Dirac-like low-energy spectrum or a very high carrier mobility, providing an effective possibility to probe the quantum phenomena. Indeed, the AB-conductance oscillations have already been observed in different graphene quantum rings (GQRs). Actually, an impressive progress in fabricating GQRs should also lead to equally notable results on the observation of the ring energy spectra and associated dynamical properties. Theoretically, the energy spectra were mainly studied for closed GQRs in the single particle approximation, using either the tight-binding method or the continuum models, where charge carriers are effectively described as massless Dirac fermions. It was shown that the energy spectra strongly depend on the ring geometry and the edge structure.

An extensively studied class of GQRs is the circular GQRs (CGQRs) that are created by an axially symmetric confinement potential such as the electrostatic potentials induced by an appro-

priate gate or a charged scanning tunnelling microscope (STM) tip. Generally, due to the Klein tunnelling, the gate/tip induced electrostatic potentials can confine carriers in just the quasi-bound states (QBSs) with a finite trapping time. Recently, Ref.[1] (J.Phys.:Condens.Matter 2016, 28, 275302; arXiv:1705. 01035) suggested the effective approaches to calculate the QBS-energy spectrum of any structure created by an axially symmetric potential in a continuous graphene sheet. On the one side, the QBS-spectrum can be extracted from the local density of states (LDOS). Each resonance emerged in the LDOS expresses a QBS with the definite resonance position (level) and resonance width. On the other side, one can directly determine the QBS-spectrum by solving the Dirac equation with an outgoing wave boundary condition. Generally, the energy spectrum is then complex: the real part and the imaginary part of a complex energy give, respectively, the resonance level and the resonance width of a QBS. And, in turn, the resonance width of a QBS measures the inverse of its trapping time. These approaches have been successfully applied to calculate the QBS-spectra of different circular graphene quantum dots.

This report is aimed at presenting the new results on the QBS-energy spectra of CGQRs that have been calculated using the approaches [1]. Calculations are carried out for the two types of CGQRs created by either a rectangular radial confinement potential or a smooth one. The QBS-spectra are in detail examined in dependence on the ring radius, the ring width, the confinement potential magnitude as well as the mass gap. Obtained results are discussed in comparison to those derived from other CGQR-models and to available experiments.

Presenter: Đinh Thị Diệu Linh

P.16 – Poster, NCTP-42

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

Nguyen Quang Hoc (1), Pham Thi Minh Hanh (2), Nguyen Ngoc Lan Anh(1) and Le Hong Viet (3)

Trường Đại Học Sư Phạm Hà Nội 2

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 moduli, 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 substitution atoms, concentration of interstitial atoms and concentration of equilibrium vacancies. The theoretical results are applied to interstitial alloy FeCrSi in the interval of temperature from 600 to 1000K, in the interval of substitution atom concentration from 0 to 10% and in the interval of interstitial atom concentration from 0 to 5%. In special cases, we obtain the thermodynamic quantities of substitution alloy FeCr, interstitial alloy FeSi and 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. Keywods: interstitial alloy, substitution alloy, statistical moment method, substitution and interstitial atoms, concentration of equilibrium vacancies.

Presenter: Lê Hồng Việt

P.17 – Poster, NCTP-42

The dynamics and structure heterogeneity in network forming liquids

N. T. T. Ha, L. V. Vinh and P. K. Hung

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The structure and dynamic in network-forming liquids has been investigated by mean of molecular dynamics simulation. Four models of silica and alumina liquids with 5500 atoms were constructed in the 2500-3500 temperature range. The structure of the silica and alumina calculated by analyzing linkage-cluster (LK- cluster). From the analysis of LK-cluster function FLKCL(r,t) and init-bond function FIB(t), the dynamics heterogeneity (DH) and its origin in network-forming liquid will be clarified. Besides, distribution of mobile and immobile clusters is also investigated via visual method. Influence of temperature on dynamical characteristics of network-forming liquids also discussed in detail.

Presenter: Nguyen Thi Thanh Ha

P.18 – Poster, NCTP-42

Calculation of the Ettingshausen coefficient in a Rectangular quantum wire with an infinite potential in the presence of an Electromagnetic wave by using a Quantum kinetic equation

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The Ettingshausen coefficient(EC) in a Rectangular quantum wire with an infinite potential (RQWIP) in the presence of an Electromagnetic wave(EMW) is calculated by using a quantum kinetic equation for electrons. Considering the case of the electron - optical phonon interaction, we have found the expressions of the kinetic tensors $\sigma_{ik}, \beta_{ik}, \gamma_{ik}, \zeta_{ik}$. From the kinetic tensors, we have also obtained the analytical expression of the EC in the RQWIP in the presence of EMW as function of the frequency and the intensity of the EMW , of the temperature of system , of the magnetic field and of the characteristic parameters of RQWIP. The theoretical results for the EC are numerically evaluated, plotted and discussed for a specific RQWIP GaAs/GaAsAl. We also compared received EC with those for normal bulk semiconductors to show the difference.The Ettingshausen effect in a RQWIP in the presence of an EMW is newly developed. Keywords: Ettingshausen effect, Quantum kinetic equation, RQWIP, Electron - phonon interaction, kinetic tensor.

Presenter: Nguyen Quang Bau

P.19 – Poster, NCTP-42

The structures of multi-period electro-weak phase transition in the 3-3-1-1 model

V. Q. Phong, N. T. Tuong, N. C. Thao, H. N. Long

Institute of Physics

The electroweak phase transition (EWPT) is considered in the framework of 3-3-1-1 model for dark matter. With a structure has many vacuum expectation values (VEVs), two VEVs on TeV scale, two VEVs on 200 GeV scale so that we approximate a phase structure has three or two periods. The first picture (two periods EWPT) has a transition $SU(3) \to SU(2)$ at 6 TeV scale and another is $SU(2) \to U(1)$ transition which is the like-standard model EWPT. The second picture is a structure of three periods EWPT which has two periods as well as the first picture and another period is the symmetry breaking process of $U(1)_N$ group. We conclude that EWPTs are the first order phase transitions when new bosons are triggers and the masses of them are about some TeVs. Especially, in two pictures, the maximum strength of the $SU(2) \to U(1)$ phase transition is equal to 2.12 so this EWPT is not strong. Moreover, neutral fermions (candidates for dark matter and obey the Fermi-Dirac distribution) can be a negative trigger for EWPT but they do not make lose the first-order EWPT at TeV scale. Furthermore, in order to the strong first-order EWPT at TeV scale, the symmetry breaking processes must produce more boson than fermion or the mass of boson must be much larger than that of fermion.

Presenter: Hoàng Ngọc Long

P.20 – Poster, NCTP-42

Distributions of neutron produced from (p,n) reaction on liquid lead target using for the accelerator driven subcritical reactor

Tran Minh Tien

Thu Dau Mot University

Accelerator driven system (ADS) subcritical nuclear reactors are under development around the world. There are many researches about (p,n) reaction for designing target, but this calculations concentrate on different types of solid target. This article in the serial of researches using liquid lead which makes not only coolant but also target and using the thorium as a fuel. This work presents the results of calculating the energy distribution, angle distribution, flux of neutron which produced as the proton beam from the accelerator interact with the target to produce (p,n) reaction. This results are the basics for designing target , calculating fuel... for the accelerator driven system subcritical nuclear reactors.

Presenter: Tran Minh Tien

P.21 – Poster, NCTP-42

Pressure-induced structural transition in supercooled liquid and amorphous silicene via molecular dynamics simulation

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An analysis of a pressure-induced structural transition in 2D amorphous and supercooled liquid Silicene is carried by MD simulations under non-periodic boundary conditions. Uncompressed supercooled liquid and a-silicene models containing 10000 atoms are obtained by rapid cooling process from the melts. Then, two models at 1000K (a-silicene) and 2000K (supercooled liquid)

have been compressed step by step up to a high density at 3.0 and 4.0 g/cm^{-3} (high-pressure condition) at constant temperature in order to observe the pressure-induced structural changes. Penta and specific mixed penta-square lattices of silicene are discovered in our calculations. Structural properties of those models have been analyzed in detail through the radial distribution functions, interatomic distances, coordination number, ring and bond-angle distributions under high pressure about 100-300 GPa. The dependence of pressure on formation behaviors are calculated via pressure-volume and total energy-density relationship. Atomic mechanism of phase transition is clarified by pressure effect on diffusion constant.

Presenter: Nguyen Truong Long

P.22 – Poster, NCTP-42

Electronic properties of superlattice structures of AlN/GaN based on armchair nanoribbons

Huynh Thi My Duyen, Lai Thi Hong Yen, Nguyen Thanh Tien

College of Natural Sciences, Can Tho University

AlN and GaN are the typical semiconductor materials. These materials were used in application for optoelectronic devices. Both AlN and GaN have crystal structure wurtzite-like and they have many similar physical properties. Therefore, these two materials are combined into superlattice, it promises to create a new material system with new physical properties. In this study, we investigate the electronic properties of the superlattice the dependent of AlN/GaN armchair nanoribbons by using the density functional theory (DFT) method. We have used the PBE functional for GGA and a plane-wave basis set with the projector augmented wave method as implemented in the Vienna ab initio simulation package (VASP). In results, it is shown that the electronic structures of some crystal structures exist the strong quantum confinement effect. Electronic properties depended on the length of segments in terms of the number of the unit cells of constituent nanoribbons (s_1, s_2) and the width in term of the number of dimer lines in the primitive unit cell of constituent nanoribbons (n_1, n_2). In AlN/GaN structures, the best strong quantum confinement effect is (9-1, 9-2) structure.

Presenter: Huynh Thi My Duyen

P.23 – Poster, NCTP-42

Develop a new tool for grading exam based on the Carbo quantum similarity and IQ curve: Application to Vietnam national exams 2012-2016

Chu Thuy Anh [1], Nguyen Tri Lan [1], Tran Cong Phong [2], Nguyen Thi Thanh Tam [3,4] and Nguyen Ai Viet [1]

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The human knowledge is deeply attached to the notion of similarity. The similarity concept was introduced in ancient Greek philosophy directly relates to the relative comparison between different systems, still nowadays plays an important role in modern natural sciences and cognitive theory. In chemical physics the quantum similarity theory was proposed by Carbo in 1980, firstly

applied to the measure of similarity between two molecules in quantum chemistry, then quickly generalized for others use in many areas of natural and social sciences. In the education, the intelligence quotient, or IQ, has a important meaning and very useful in practices. The IQ score distribution curve is well established and wildly recognized. In this work, we propose a new tool for quantitative grading the succeed of the exam using the Carbo quantum similarity and IQ curve. Considering that the well exam result is good if its score distribution is maximal similarity with IQ curve, the susceptibility of the exam can be graded in spirit of the Carbo index. As an example, we apply our method for investigation and grading the Vietnam national exams in the period 2012-2016.

Presenter: Chu Thuy Anh

P.24 – Poster, NCTP-42

Coherent potential approximation study of the three component Falicov-Kimball model

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We study the paramagnetic phase diagram in a three-component Falicov-Kimball model within the coherent potential approximation. The model can be realized in an optical lattice at ultra-low temperature as a mixture of two interacting fermion atom species. One species is immovable single-component atoms, in contrast, the other species is movable two-component atoms. Depending on the atom filling conditions and local interaction strength, different correlation-driven metal-insulator transitions are observed. These metal-insulator transitions are investigated by monitoring the density of states at the Fermi level and the energy gap. Although our approach is analytically simple and numerically fast, the obtained results are in good agreement with the ones obtained by much more sophisticated theory. Keywords: three-component Falicov-Kimball; Metal-insulator transitions

Presenter: Nguyễn Thị Hương

P.25 – Poster, NCTP-42

Drude-jellium model for microwave conductivity of electrolyte solutions

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Characterization of static conductivity of electrolyte solutions at microwave frequencies plays an important role in fundamental process of biology and chemistry, for examples, electrokinetic phenomena, charge transfer in living cell, electrolysis. Recently, the microwave conductivity of the salt solution was determined with a rather accuracy by measuring its dielectric constant on the basis of combination between the Debye and Drude models. In this work, we consider that the electrolyte solution is a plasma consisting of ions with water background. Using the jellium

theory, its plasmon frequency is calculated. Moreover, we can provide the relation to determine the static conductivity of the electrolyte solutions by the combination between this plasmon relationship and the Drude formula for dielectric constant. Our approach gives a good agreement between calculations and experimental data. We can estimate the value of the damping coefficient for the conductive solutions at low frequencies. Our study also predicts the microwave conductivity for a variety of salts with a wide range of concentrations by using the microfield approach.

Presenter: Tran Thi Nhan

P.26 – Poster, NCTP-42

Melting of Two-Dimensional Crystal with Square Lattice Structure

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We present the molecular dynamic (MD) simulations of melting of two-dimensional (2D) crystal with the square lattice structure. Model contains 6400 atoms interacted via the square potential proposed by Rechtsman et al. (Phys. Rev. E, 2006, 73, 011406). The model is heated up from 0.1 to 1.0 (in reduced Lennard-Jones unit) in order to show the evolutions of various thermodynamic properties and structural characteristics. We find that the spontaneous melting of the 2D model exhibits the first-order behavior of the transition from the square lattice structure to the 2D liquid-like triangle lattice structure. Various structural and thermodynamic properties upon heating from the solid state to the liquid state are analyzed in details via radial distribution functions, temperature dependence of total energy and heat capacity, coordination number distributions, ring statistics, bond orientation orders, interatomic distances and bond angle distributions. The heat capacity of the system exhibits a single peak that exists at around the melting point . Atomic mechanism of melting is analyzed via monitoring the spatio-temporal arrangement of the liquid-like atoms occurred during the heating process. This research is funded by Vietnam National University Ho Chi Minh City (VNU-HCM) under grant number B2017-20-02.

Presenter: Le Nguyen Tue Minh

P.27 – Poster, NCTP-42

Effects of macromolecular crowding on the escape of nascent proteins from the ribosomal tunnel

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After being fully synthesized, nascent proteins must travel through the ribosomal exit tunnel before entering an environment crowded by other proteins and molecules. Both the confinement of the tunnel and the crowding of the intracell environment are known to significantly alter protein folding behaviors, but they are often considered separately in theoretical and simulation

studies. In this work, by using coarse-grained models with Langevin dynamics, we simulate the folding and escape of nascent proteins in presence the both the tunnel and the macromolecular crowders outside the tunnel mimicking more closely what happens in the cells. We find that the crowders slow down the escape process. Like for the case without crowders considered in our previous study, the escape time of protein remains to be well fitted by a simple diffusion model. We analyze the dependence of the effective diffusion constant of proteins on temperature and on the crowders' volume fraction and illustrate the impact of macromolecular crowding on the dynamics of nascent proteins at the ribosomal tunnel.

Presenter: Bui Phuong Thuy

P.28 – Poster, NCTP-42

Improvement the quantum teleportation via pair coherent states

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In this paper we present two methods to improve the quantum teleportation processes for teleporting a coherent state via the pair coherent states. In our protocols, we use the measurement of the orthogonal quadrature components, and the photon number sum and phase difference. In the first protocol, we add a displacement of photon number at receiver and indicate measurement of probability in the second protocol. In the two methods mentioned above, our results show that the average fidelities approach to unit depending on the parameters involved.

Presenter: Truong Minh Duc

P.29 – Poster, NCTP-42

Investigating the Influence of Dynamic-Core Polarization on High-Order Harmonics of Linear Molecules

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

Using single active electron potential, we develop a method to calculate the high-order harmonics spectra for molecules by solving the time dependent Schrodinger equation within single active electron approximation. Firstly, the dependence of harmonics spectra on orientation of molecules in an ultrashort laser is presented. Then, taking into account the interaction of the active electron with the core electron induced by the laser, we theoretically investigate the influence of dynamic core polarization on high-order harmonic generation of polar (CO) and nonpolar (CO2) molecules.

Presenter: Le Thi Cam Tu

P.30 – Poster, NCTP-42

Magneto-optical absorption and cyclotron-impurity resonance in silicene

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(1) University of Education, Hue University; (2) The Vietnam Institute of Educational Sciences

The optical absorption of Dirac fermions in silicene, subjected to a perpendicular magnetic

field, is study by the perturbation theory. Analytical expression of the absorption coefficient is obtained taking account the electron - impurity interaction at very low temperatures. Absorption spectra show the appearance of cyclotron-impurity resonant peaks. The dependences of the absorption coefficient on the magnetic field and temperature are also obtained and discussed.

Presenter: Le Thi Thu Phuong

P.31 – Poster, NCTP-42

Anomalous Velocity by Berry Curvature Effect in Semiconductor GaAs Quantum Well

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The anomalous movement of charge carriers in solids subjected to an electric driving field is one of the most intriguing properties. Their velocity has a perpendicular component to the electric field, even without any magnetic field. There are two types contributing to anomalous velocity: intrinsic effect linked to Berry curvature, and extrinsic effect due to scattering processes, known as skew scattering and side jump. In this work, we focus on studying the intrinsic effect caused by Berry curvature. Firstly, using kp14 method, we get the band structure of GaAs quantum well. Then, the anomalous current of charge carriers can be obtained by solving semiconductor Bloch equation with a terahertz laser.

Presenter: Ngô Thành Công

P.32 – Poster, NCTP-42

Molecular Dynamics Simulation of Melting of 2D Glassy Monatomic Systems

Duong Thi Nhu Tranh, Vo Van Hoang

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Melting of 2D glassy monoatomic systems is studied via molecular dynamics (MD) simulations. 2D glassy models are obtained by cooling from the melt and then are heated with Lennard–Jones–Gauss (LJG) interaction potential. Temperature dependence of various structural and dynamical properties of the systems during heating is analyzed and discussed via partial radial distribution functions (PRDFs), coordination number distributions, ring statistics, mobility of atoms and their clustering. We found a transition temperature region, in that structural and dynamical properties of systems strongly change. In addition, we also found that fraction of atoms with very low mobility (solidlike ones) decreases with increasing temperature down to zero. This research is funded by Vietnam National University - Ho Chi Minh City (VNU-HCM) under grant number B2017-20- 02.

Presenter: Duong Thi Nhu Tranh

P.33 – Poster, NCTP-42

Investigation of magneto-phonon resonance in graphene monolayers

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In this work, utilizing the linear response theory we calculate the magneto-conductivity (MC) in graphene monolayers, subjected to a static perpendicular magnetic field. The interaction of Dirac fermions with optical phonon via deformation potential is taken into account at high temperature. The dependence of the MC on the magnetic field shows resonant peaks that describe transitions of electrons between Landau levels via the resonant scattering with optical phonons. The effect of temperature on the MC is also obtained and discussed.

Presenter: Bui Dinh Hoi

P.34 – Poster, NCTP-42

Interplay between disorder, magnetism and topology in topological insulators doped with magnetic impurities

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A topological insulator doped with random magnetic impurities is studied. The system is modelled by the Kane-Mele model with a random spin exchange between itinerant electrons and magnetic impurities. The dynamical mean field theory is used to investigate the electron dynamics. Both magnetic long-range order and the Hall conductance are calculated. They reveal a rich phase diagram, where various magnetic long-range orders such as the antiferromagnetic or ferromagnetic ones can exist in the topological insulator phase, depending on the electron and magnetic impurity concentrations as well as the ratio between the spin exchange and the spin-orbit coupling.

Presenter: Nguyen Hong Son

P.35 – Poster, NCTP-42

In Silico Study of Bombyx Mori Fibroin Enhancement by Graphene

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Recently, by feeding the silkworms with graphene, the obtained fibroin after feeding shows the incredible improvement in either mechanical properties or electrical conductivity [Q. Wang et al., Nano Lett. 16, 6695 (2016)]. Moreover, their Raman spectra and transmission electron microscopy show the evidence of carbonization of the silk fibers. However, the interaction between fibroin and graphene has not been thoroughly understood. Therefore, in this work, we used molecular dynamics simulation to shed light on the interaction between Bombyx Mori Fibroin and graphene fragment. We found that the negatively charged residues play the role of keeping the contact with graphene while TYR and PHE play the role of guiders for graphene to find

the stable binding site. In addition, we performed QM/MM optimization for the obtained complexes. The results contribute to answer the enhancement of silk fiber via carbonization with graphene.

Presenter: Tran Thi Thu Hanh

P.36 – Poster, NCTP-42

Cosmic inflation in modified gravity f(R) of polynomial – exponential form

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In this paper, we investigate cosmic inflation in modified gravity f(R) of polynomial – exponential form. The cosmic inflation is driven by a scalar field induced in the modified gravity. Results show that cosmic inflation puts a strict constraint on the parameters of the model: parameter of alpha less than 10 power (-46) . Reheating after cosmic inflation in the model also investigated.

Presenter: Vo Van On

P.37 – Poster, NCTP-42

Simulations properties dynamics in $Al_2O_3.2SiO_2$

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(1) Thu Dau Mot University;(2) Institute of Applied Materials Science; (3) Ton Duc Thang University

This paper presents the results of studying the dynamic properties of Al2O3.2SiO2 through change the size of O-simplex and T-simplex in the pressure range from 0 GPa to 25 GPa by molecular dynamics method with the interaction Born - Mayer. The simulation was performed on a 1998 atomics models to clarify the diffusion mechanism in Al2O3.2SiO2.

Presenter: Mai Van Dung

P.38 – Poster, NCTP-42

Adsorption of CO_2 in metal organic framework of MIL-88a by computational methods

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Carbon dioxide (CO2) is a main gas causing the greenhouse effect and global warming. Therefore, the minimization of CO2 emissions is an important task. Many studies of CO2 capture by using metal organic frameworks have been performed. MIL-88A has a high flexibility and stability. However, there are no available works for the study of the CO2 capture in MIL-88A. In this work, density functional theory and grand canonical Monte Carlo simulations were applied to elucidate the CO2 adsorption in MIL-88A and assess the CO2 capture ability of MIL88A. Our results are quite remarkable and can be used as a reference for experiments.

Acknowledgement. This research was funded by Ho Chi Minh City University of Technology under grant number SVCQ-2016-KHUD-31.

Presenter: Son Do

P.39 – Poster, NCTP-42

A Tsallis entropy–based thermodynamic description of ecological systems

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It has been proved that non–extensive entropy (Sq) proposed by Tsallis for statistical physics would be considered as generalized formally equivalent version of biodiversity index which covers several other well–know versions of biodiversity indices such as Shannon–Wiener (H), Simpson (D). Moreover, a Tsallis entropy–based thermodynamic theory for ecological systems would have been constructed by the standard routines of statistical physics to determine the most important ecologically physical quantities such as ecological internal energy (Uq) and temperature (Tq). Within this proposed approach, an opportunity to build up a full thermodynamic description of ecological systems would be ready in all possible aspects. This work presents in details the method and accompanied technique to realize this idea and discusses the ecological and physical consequences of obtained results.

Presenter: Le Van Xuan

P.40 – Poster, NCTP-42

A model for enhancement factor and selection ruler of Surface Enhanced Raman Scattering

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Surface-Enhanced Raman Spectroscopy or Surface-Enhanced Raman Scattering (SERS) is a new surface-sensitive technique that enhances Raman scattering by molecules adsorbed with a huge enhancement factor 1014-16. Therefore, SERS has a great attention on both theory and experiment in many fields as chemistry, physics, materials science, nano-science, and the life sciences. In this work, we propose a new model to explain the huge enhancement factor and the non-usual optical selection rule of SERS. In understanding the mechanism of huge enhancement effect, beside the chemical theory with the formation of charge-transfer complexes, we concentrate our attention to the electromagnetic mechanism with surface plasmon polariton effect. The non-linear electric field mechanism for optical selection ruler also assumed and discussed.

Presenter: Duong Ha

P.41 – Poster, NCTP-42

Energy of exciton in monolayer semiconductor WS2 with taken into account of modified Yukawa screening potential

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(1) AMOG, Research Group, Ton Duc Thang University; (2) Physics Department, Ho Chi Minh City University of Pedagogy

The Yukawa screening potential is modified to describe the effect of environment on energy of exciton in monolayer semiconductor WS2. The FK Operator Method combined with Laplace transformation is used to retrieve the energies for the states of n= 1, 2, 3 which are coincident with experimental data. Experimental values of the parameters in the screening potential expression are also obtained for further use in the case of presence of external field.

Presenter: Hoang Do Ngoc Tram

P.42 – Poster, NCTP-42

The photon-drag effect in cylindrical quantum wire with an infinite potential for the case of electrons–acoustic phonon scattering

Hoang Van Ngoc (1), Nguyen Vu Nhan (2), Hoang Dinh Trien (3), Nguyen Quang Bau (1)

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The photon - drag effect with electrons – acoustic phonon scattering in cylindrical quantum wire with an infinite potential is studied. With the appearance of the linearly polarized electromagnetic wave, the laser radiation field and the dc electric field, analytic expressions for the density of the direct current are calculated by the quantum kinetic equation. The dependence of the direct current density on the frequency of the laser radiation field, the frequency of the linearly polarized electromagnetic wave and the temperature of the system is obtained. The analytic expressions are numerically evaluated and plotted for a specific quantum wire, GaAs/AlGaAs. The difference of the density of the direct current in quantum wires from quantum well and bulk semiconductor is due to potential barrier and characteristic parameters of system. These results are for every temperature and are new results.

Presenter: Hoang Van Ngoc

P.43 – Poster, NCTP-42

Using generalized Bogoliubov transformation to study the collective behaviors of social complex systems

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In the theoretical physics Bogoliubov transformation is well–known as an effective method for investigating systems consisted of two kinds of interacting particles. However, the application of the Bogoliubov transformation would not be limited only in the studying physics, but also be extended and applied to study a number of complex systems modeled by quasi–Hamiltonians. This transformation provides a simple methodology in research of complex systems and allows to obtain richer awareness of the collective behaviors that are universal in such complex systems. In the view of the formal equivalence (isomorphism) between many body physical systems

and multi–agent complex systems, the use of approaches well–developed in the physics to study collective behaviors of the groups, the communities offers reliable and convincible results and might be considered as an inevitable tendency, complementing the shortcomings of the traditional mathematical tools in the study of complex systems. This study is one of the efforts to introduce a physical tool to study the most interesting and simple phenomenon in social complex systems, teachers in a classroom, transition from Boltzmann distribution to Gaussian one.

Presenter: Chu Thuy Anh

P.44 – Poster, NCTP-42

The DFT Study of the Hydrogen Electroadsorption on the Missing Row Pt(110)-(1×2) Surface.

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The hydrogen adsorption isotherms are reported on the missing row Pt (110)-(1×2) within the conventional ultrahigh vacuum (UHV) surface modeling. They are evaluated by the combination of the density functional theory (DFT) and the Monte Carlo (MC) simulations. The binding energy for adsorption is found to depend strongly on the hydrogen coverage. The short bridge sites on the ridge (R) are found to be the strongest binding sites at low coverage. At a higher H coverage, up to 1ML, the on-top sites of the micro-facet (F) get populated. The relative abundance of the H_R and H_F are investigated. The influence of the exposed ridge atoms on the adsorption properties are found to be negligible at 1/3 ML, and the presence of the trough atoms have the most influence at the intermediate coverage.

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Presenter: Tran Thi Thu Hanh

P.45 – Poster, NCTP-42

Investigation of hydrogen adsorption in M(bdc)(ted)$_{0.5}$ by computer simulation methods

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Finding new energy sources replacing for fossil fuels is an urgent need. In addition, the new energy carrier has to be clean and environmentally friendly to prevent pollution. Hydrogen gas is believed to be an excellent candidate due to its advantages in comparison with other fuels. However, hydrogen gas storage is a difficult issue. A number of materials have been studied to store hydrogen gas such as zeolite, activated carbon, silica gel, etc. Among the studied materials, the metal organic framework (MOF) is most promising for hydrogen storage because of its exceptionally high surface area and ultra-large pore size. Computer simulations allow the prediction and design of new MOF structures with a significant storage capacity of hydrogen gas in recent years. In this report, we use density functional theory and grand canonical Monte Carlo methods to explore the electronic structure properties, adsorption energies, and hydrogen loadings in M(bdc)(ted)$_{0.5}$.

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Presenter: Nguyen Thi Xuan Huynh

P.46 – Poster, NCTP-42

Problem of transition between Gaussian-like and Boltzmann-like forms of envelope functions in atomic and condensed mater physics

Man Van Ngu (1), Ngo Gia Vinh (2), Chu Thuy Anh (3), Truong Thi Ngoc Anh (4,5), Nguyen Tri Lan (3), Nguyen Ai Viet (3).

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The transition between Gaussian-like and Boltzmann-like forms of probability functions or statistical envelope functions are quite common in complex systems. This form changing of stock exchange returns in time, and envelope function of a Cooper pair in space variables are shown in the our previous works. In this work we continue investigate this form transition in the problem of presence of strong magnetic field in atomic and condensed mater physics. Following the famous Einstein's idea about the connection between interaction and geometry of vacuum, these form transition can be attributed to an effective changing of vacuum symmetry of systems.

Presenter: Mẫn Văn Ngữ

P.47 – Poster, NCTP-42

In silico Studies of Solvated F19W Amyloid β (11-40) Trimer

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The role of F19 residue and the effect of its mutations on amyloid beta trimer (3Aβ), which was recently shown to be one of the most toxic amyloid beta oligomers, have not been addressed. Here we extensively studied the F19W mutant of 11-40 truncated 3Aβ (F19W 3Aβ 11-40) using REMD simulations over 19.2 μs in total. F19W 3Aβ 11-40 forms slightly different secondary structure terms compared to 3Aβ 11-40. The beta structure content slightly increase by 3% while the coil content decreases by 3%. The distributions of these terms per residue also shift. Critical intermolecular polar contacts (D23 to V24, G25, S26, N27, and G29) intermolecular polar contacts (H13A-Q15B and H13B-Q15C) of F19W 3Aβ11-40 decrease significantly, while only the salt bridge D23-K28 is enhanced. Solvent accessible surface area (SASA), radius of gyration (Rg), and number of contacts do not change to a significant extents; however, RMSD almost doubles upon F19W mutation. Six minima were found in the free energy surface of F19W mutant, which have slightly lower energy barriers (by $\sim$ 1 kJ/mol) and significantly lower total population (20%) compared to those of the three minima previously found for 3Aβ11-40 (60%). The binding free energy between constituting chains of the mutant trimer increases by $\sim$ 28 kcal/mol but fluctuates significantly ($\pm$ 27.1 kcal/mol). Our results indicate that while the

hydrophobic core of Aβ peptide is capable adapting to changes, F19W mutation results in a significantly more dynamic trimer that would require more time to self-assemble into fibrils according to experiments.

Presenter: Ngo Son Tung

P.48 – Poster, NCTP-42

Pressure-induced structural transition in supercooled liquid and amorphous-silicenevia molecular dynamics simulation

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An analysis of a pressure-induced structural transition in 2D amorphous and supercooled liquid Silicene carried by MD simulations under non-periodic boundary conditions. Uncompressed supercooled liquid and a-silicene models containing 104 atoms are obtained by rapid cooling process from the melts. Then, two models at 1000K (a-silicene) and 2000K (supercooled liquid) have been compressed step by step up to a high density at 3.0 and 4.0 g/cm-3 (high-pressure condition) at constant temperature in order to observe the pressure-induced structural changes. Penta and specific mixed penta-square lattices of silicene are discovered in our calculations. Structural properties of those models have been analyzed in detail through the radial distribution functions,interatomic distances, coordination number, ring and bond-angle distributions under high pressure about 100-300GPa. The dependence of pressure conformation behaviors are calculated via pressure-volume and total energy-density relationship.Atomic mechanism of phase transition is clarified by pressure effect on diffusion constant.

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Presenter: Huynh Anh Huy

P.49 – Poster, NCTP-42

One loop corrections to decay $h^0 \to l_a l_b$ in economical 3-3-1 model

L. T. Thuy (1), V. N. Hien (1), P. H. Dinh (1), T. Phong Nguyen (1), L. T. Hue (2)

(1) Can Tho University; (2) Institute of Physics

Lepton Favor violating (LFV) decays, i.e the decays of the standard like-Higgs boson such as $h^0 \to l_a l_b$ is investigated. In the limit of the unitary gauge, one-loop contributions to the branching ratio $BR(h^0 \to l_a l_b)$ is shown in the framework of the economical 3-3-1 (E331) model

Presenter: Le Thu Thuy

P.50 – Poster, NCTP-42

Plasmon modes in Dirac/Schrödinger hybrid electron systems including layer-thickness and exchange-correlation effects

Nguyen Van Men (1,2), Nguyen Quoc Khanh (2)

(1) University of An Giang; (2) University of Science - VNUHCM

We calculate the plasmon dispersion relation and damping rate of collective excitations in a double-layer system consisting of monolayer graphene and GaAs quantum well at zero temperature including layer-thickness and exchange-correlation effects. We use the generalized random-phase-approximation dielectric function and take into account the nonhomogeneity of the dielectric background of the system. We show that the effects of layer thickness, electron densities and exchange-correlations are more pronounced for acoustic modes, while the optical branch depends remarkably on dielectric constants of the contacting media.

Presenter: Nguyễn Văn Mện

P.51 – Poster, NCTP-42

The crystallization of liquid iron nanoparticles

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The crystallization of liquid iron nanoparticles has been investigated by means of molecular dynamic (MD) simulation. Simulation result shows that when the liquid samples are cooled from 2500K to 300K at a cooling rate of 0.667K/ps, they are crystallized into body centered cubic (bcc) phase. The transformation to crystalline phase is analyzed through the Common Neighbor Analysis (CNA) methods. The crystallization is carried through two processes: the transformation from liquid to icosahedrons (ico) structure and the transformation from ico to bcc structure. Further, we focus on the size dependence of crystallization of liquid iron.

Presenter: Nguyen Thi Thao

P.52 – Poster, NCTP-42

Surface optical phonon-assisted cyclotron resonance in monolayer phosphorene on polar substrates via two photon absorption process

Huynh Vinh Phuc (1), Luong Van Tung (1), Le Dinh (2)

(1) Dong Thap University; (2) Hue University's College of Education

We theoretically study the influence of surface optical (SO) phonons on the phonon-assisted cyclotron resonance (PACR) effect in a monolayer phosphorene 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 effects of polar substrates on the MOAC and full-width at half maximum (FWHM) through their electron-SO phonon scattering are presented. We also discussed the effects of temperature, phosphorene-substrate thickness, and magnetic field on the MOAC and the FWHM. The present results for monolayer phosphorene are compared with those in conventional two-dimensional systems as well as in graphene. Our results provide a significantly quantitative picture for SO phonon interaction induced magneto-optical absorption in phosphorene on polar substrates.

Presenter: Huỳnh Vĩnh Phúc

P.53 – Poster, NCTP-42

Spinor Tachyon of Gravitational Origin

Dao Vong Duc (1), Phu Chi Hoa (2)

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In the framework of the concept of generally covariant duality introduced introduced in the previous work/D V Duc and P C Hoa, J. of Modern Phys. Vol 5, P 2016 (2014)/ we consider the possibility for the existence of spinor tachyon fields which are closely related to scalar tachyon fields of cosmological nature with masses expressed by Einstein cosmological constant.

Presenter: Dao Vong Duc

P.54 – Poster, NCTP-42

Some application of q-deformed energy spectrum inverse problem and observer entanglement model of composite bosons

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Energy spectrum inverse problem and observer entanglement model of composite bosons was investigated in our previous works. We have proposed deformed-three-levels simple model, where the set-parameters of level deformations are easily and explicitly defined. Using deformed-three-levels simple model with observer effect, we introduced the outside and inside looking entanglements of composite bosons. This observer definition of entanglement gives a new tool for studying the connection between the deformation energy levels of a boson and the effect of surrounding environment. In this work, we demonstrate some application of our model for physical systems: hydrogen atom, exciton, diatomic molecules, Copper pairs, and system in a closed box.

Presenter: Nguyen Anh Sang

P.55 – Poster, NCTP-42

Effect of exact thermal pairing on nuclear level density of even-even nuclei

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Nuclear level density (NLD) is studied within a microscopic approach, which is derived based on the exact thermal pairing (EP) of the pairing Hamiltonian for the truncated single-particle levels around the Fermi surface in combination with the independent-particle model (IPM) for the single-particle levels outside the truncated space [1]. The numerical calculations are carried out for various even-even nuclei, whose experimental data are available. The results obtained show that EP is indeed very important for the valid description of NLD in the low and intermediate regions of excitation energy.

[1] N. Quang Hung, N. Dinh Dang, and L. T. Quynh Huong, Phys. Rev. Lett. 118, 022502

(2017).

Presenter: Le Thi Quynh Huong

P.56 – Poster, NCTP-42

Cooling rate effect and size effect on formation of two-dimensional SiC from the liquid state

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We present molecular dynamics (MD) simulations of formation of SiC from liquid state. The initial systems (containing 3000 and 9968 atoms Si and C) are arranged a planar with honeycomb structure and under periodic boundary conditions. The particles in the models interacted via Tersoff potential (Phys. Rev. B 39, 5566, 1989). Models are heated to temperature much higher melting point in order to get liquid state. Then, models are cooled down to 300 K. Evolution of structure and thermodynamic properties upon cooling/heating are found and discussed such as radial distribution functions (RDF), temperature dependence of total energy, potential and kinetic energy, volume and mass density, ratio between volume at given temperature and initial volume, bond-angle distribution, interatomic distance between Si-C, Si-Si and C-C bonding, ring size distribution, mean of coordination number Si (total), C (total) and partial coordination number Si(C), Si(Si), C(Si), C(C). 2D visualization of atomic configurations are also presented. Formation of 2D-SiC from the liquid state has been effected by size of model and cooling rate. The atoms with a same style have a tendency to aggregate into clusters, we find the existence of some small graphene (formation of species of only C-C binding in honeycomb structure) and silicene domains in the models of SiC obtained at 300 K (formation of species of only Si-Si binding in honeycomb structure). All the models received at 300 K are amorphous SiC.

Acknowledgements: This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under Grant 103.02-2016.88.

Presenter: Truong Quoc Tuan

P.57 – Poster, NCTP-42

Tuning Electronic Properties of Transition Metal Dichalcogenides Monolayer by Polymer Doping

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Recently, two-dimensional transition metal dichalcogenides (TMDCs) materials have been widely studied due to their unique electrical, optical, and mechanical properties. Tuning the electronic properties of TMDCs is essential for improving transistor performance in nanoelectronics devices. In this study, we demonstrate the effect of polymer doping on TMDCs monolayer by using density functional theory calculations. Our results show that after polymer doping the width of the band gap of TMDCs monolayer decreases significantly compared to without polymer doping. The results can be explained through analysis of the density of state of the monolayer.

Presenter: Ong Kim Le

P.58 – Poster, NCTP-42

Cyclotron resonance linewidth in quantum wells with different phonon models

Nguyen Dinh Hien (1), Le Dinh (1), Vo Thanh Lam (2), Tran Cong Phong (3)

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The influence of different phonon models on the cyclotron resonance (CR) effect and CR linewidth (CRLW) via photon absorption processes in a square quantum well by using the operator projection is theoretically studied. We consider the cases when electrons are scattered by bulk phonons and confined optical phonons described by the Fuchs-Kliewer slab, Ridley's guided, and Huang-Zhu models. The numerical result for a specific quantum well shows that the CRLW increases with temperature, magnetic field and decreases with well's width for all the phonon models. It is also seen that CRLW in the cases of confined phonons described by all three models (HZ, slab mode, and guided mode) varies faster and has a larger value than it does for the bulk phonons case. Besides, the CRLW is found largest for HZ model among the three confined phonons models, while it is smallest for guided mode model case. This renders that the electron-confined phonon scattering is strongest for HZ model and weakest for guided mode model. Furthermore, in the small range of the well's width, the influence of phonon confinement plays an important role and cannot be neglected in considering CRLW. The present results are in qualitative agreement with the existing theoretical and experimental results.

Presenter: Nguyen Dinh Hien

P.59 – Poster, NCTP-42

Polar charges effect on multisubband electron mobility and linear intersubband optical absorption in the semiparabolic quantum wells based on AlN/AlGaN/AlN

Nguyen Thanh Tien (1), Nguyen Nhut Tuan Hung (1), Tieu Tin Nguyen (1), Pham Thi Bich Thao (1,2)

(1) Can Tho University; (2) Graduate University of Science and Technology, Vietnam Academy of Science and Technology

This work presents multisubband electron mobility and linear intersubband optical absorption in the polarization semiparabolic quantum wells (SPQWs) AlN/AlxGa1–xN/AlN. First, a theory of multisubband mobility and the intersubband optical absorption between the lowest two subbands under a uniform external electric field is studied. By using the variation method, the one-dimensional Poisson and Schrodinger equations have been solved within a finite potential barrier model and a bent band figured by all confinement sources (realistic model). Then, we computed and discussed about the effective confining potential profile, the wave function and the distribution of electron gas in quantum wells, multisubband mobility and intersubband optical absorption coefficient. Our result shows that the positive interface polarization charges effect on the distribution of the two-dimensional electron gas (2DEG) in SPQWs so it has great influences on multisubband mobility and the total optical absorption coefficients.

Presenter: Pham Thi Bich Thao

P.60 – Poster, NCTP-42

Study of Influence of the anharmonic effect on changing size and shape of the material with the cubic crystal structure by an analytic statistical moment method.

Cao Huy Phuong

Physics Unit, Faculty of Maths - Informatics, Hung Vuong University

Vibrations of atoms or ions around the lattice points are inhamonic that cause the thermodynamic effects for the materials with the crystal structure. Using the moment statistical method in the statistical physics, within the fourth order moment approximation, we have found out that the change of the length, volume and shape of the material with the cubic crystal structure are determined by the anharmonic effect. Increasing temperature leads to the more strong anharmonic lattice vibrations that cause changing size of the material.

Presenter: Cao Huy Phuong

P.61 – Poster, NCTP-42

The electronic transport properties of the zigzag graphene nanoribbons

Vo Trung Phuc (1), Nguyen Van Ut (1), Bui Thai Hoc (1) and Nguyen Thanh Tien (1)

College of Natural Science, Can Tho University

Density-functional theory (DFT) in combination with the nonequilibrium Green's function formalism is used to study the effect of substitutional doping on the electronic transport properties of zigzag graphene nanoribbons (ZGNRs). We study the various edge structures passivated by H atoms and by P atoms. In this work, Si atoms are used to substitute C atoms located at the edge or the centre of the samples. We consider 8-ZGNRs, 12-ZGNRs and 16-ZGNRs respectively. Our calculated results have determined that the electronic transport properties of the single Si-doping structures are better than the double doping ones. Moreover, there is significantly difference in the transmission spectrum of P-passivated ZGNRs and H-passivated ZGNRs i.e. P passivation does not possess an enhanced transmission at the Fermi level, which are typical for graphene nanoribons. The relationship between the transmission spectrum, the device density of states and the I-V curve indicates that P-passivated ZGNRs can stably exist in experiment and be applied well in nanodevices. We also carry out research ZGNRs with the distortion. The studied results shown that the strong transmission at the Fermi level in the perfect ribbon is also present in the distorted ribbon. Apart from this, the transmission spectra for the distorted GNRs are strongly suppressed due to scattering by the distortion.

Presenter: Nguyen Thanh Tien

P.62 – Poster, NCTP-42

High-order harmonic generation from excited hydrogen molecular ion

Phi-Hung Tran, Van-Hung Hoang, Ngoc-Loan Phan

Department of Physics, Ho Chi Minh City University of Education

High-order harmonic generation (HHG) spectra emitted from hydrogen molecular ion prepared in

the ground and the two first excited states are systematically studied by numerically solving time dependent Schrödinger equation. We demonstrate that the ratio of HHG intensity from these three lowest states is strongly sensitive to the intensity of the laser field. Importantly, influence of ionization probability and depletion phenomenon HHG are also analyzed. We have showed a closely relation between the HHG efficiency and the quantity $\gamma(t)$, which is proportional to the recombination process. Beside, the depletion effect also leads to reducing the cutoff frequency from its prediction in HHG spectra by three-step-model model.

Presenter: Phan Thi Ngoc Loan

P.63 – Poster, NCTP-42

Dependence of Short-Channel Effects on Semiconductor Bandgap in Tunnel Field-Effect Transistors

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(1) Dalat University; (2) National Chi Nan University

Using low-bandgap materials is considered as an effective method to enhance the performance of tunnel field-effect transistors (TFETs). Based on two-dimensional simulations, the dependence of short-channel effects on the semiconductor bandgap in TFETs is examined in this study. Even though the supply voltage is decreased in parallel with the bandgap, simulation results show that the short channel effect is more severe with using lower bandgap semiconductors. For a given bandgap material, the short-channel effect can be well evaluated by the variation of drain-induced barrier thinning (DIBT) with decreasing the channel length. For TFETs using different bandgap materials, however, their short-channel effects cannot be compared properly by comparing the DIBTs. Adequately considering the effect of bandgap on the short-channel performance of TFETs is important in designing extremely scaled integrated circuits.

Presenter: Nguyễn Đăng Chiến

P.64 – Poster, NCTP-42

Computer simulation of phase separation in 2D binary Lennard-Jones system

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In this study, we present the microphase separation of two-dimensional (2D) binary Lennard-Jones system studied via molecular dynamics (MD) simulations. Models are cooled from liquid to glassy state in order to see the onset of phase separation. Models contain 8100 particles with identical size and interaction parameters σ_{11}, σ_{12}, σ_{22}, ε_{11}, but different ε_{12}, ε_{22}, interacted via Lennard – Jones potential of binary systems introduced by Kob-Andersen [1]: $U(r) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right]$ Dependence of various thermodynamic properties on different ratios $\varepsilon_{12}/\varepsilon_{22}$ is analyzed in details via radial distribution function (RDF), temperature dependence of total energy and mean cluster size. Microphase separation is monitored via 2D visualization of atomic configurations at various temperatures upon cooling from the melt using VMD software. We find that the speed of microphase separation process and cluster shapes depend on the ratio $\varepsilon_{12}/\varepsilon_{22}$. The appearance of stripe patterns occurs when ε_{12} is larger than ε_{22} (the ratio $\varepsilon_{12}/\varepsilon_{22}$ is larger than 1) and the separation process is difficult to observe. In contrast, the bubble phases

are characteristic of systems with ε_{12} is smaller than ε_{22} (the ratio $\varepsilon_{12}/\varepsilon_{22}$ is smaller than 1) so it is easy to observe the microphase separation process.

Presenter: Duong Thi Nhu Tranh

P.65 – Poster, NCTP-42

Structural and electronic properties of amorphous TiO_2 nanoparticles

Le Thi Hong Diep (1), Ca Nguyen Anh Khoa (1), Huynh Anh Huy (2), Phan Thanh Hung (3)

(1) College of Natural Sciences, Can Tho University, Vietnam; (3) School of Education, Can Tho University, Vietnam; (4) Department of Materials Science, Tra Vinh University, Vietnam.

Density Functional based Tight-Binding (DFTB) method was used to study the structural and electronic properties of six amorphous TiO_2 nanoparticles (a-TiO_2) with different sizes and shapes. Initial models were cut from the anatase and rutile bulk. Then, all dangling Oxygen, some other Titanium and Oxygen atoms were removed to ensure that Ti:O ratio was 2:1. To received the amorphous TiO_2 nanoparticles, the initial models have been annealed from 0 K to 2250K in the linear ramp of 10 ps, followed by equilibration at the constant temperature of 2250 K for 5 ps and cooled down 0 K with an exponential ramp of 15 ps. Structural and electronic properties have been investigated via the Radial Distribution Functions (RDF), coordination number, surface energy and Density Of State (DOS). The findings show that the splitting in RDF of Ti-Ti pair similar to other research about a-TiO_2 and the presence of undercoodinate Ti atoms on the surface. The density of state reveal that all a-TiO_2 have lower energy gaps than those of crystalline phases, the tail states at the valence band edge are due to the appearance of 2-fold coordinate O atoms; whereas, the tail states at the conduction band edge are localized on 4-fold coordinate Ti atoms. Finally, the research also indicates that the surface energy and the band gap of a-TiO_2 strongly depend on their size and shape.

Presenter: Ca Nguyễn Anh Khoa

P.66 – Poster, NCTP-42

Theoretical investigation of quantum beat of excitons in GaAs/AlGaAs quantum wells

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College of Education, Hue University

In this paper, we studied theoretically the quantum beat of excitons in GaAs/AlGaAs quantum wells using renormalized wavefunction formulation of a three-level energy diagram. We observed the quantum beat of excitons while there was being a strong laser coupling two electron quantized levels. Quantum beat is observed at twice the electron Rabi frequency. In addition, we found dependences of intensity of absorption of the quantum beat of excitons on wells length and pump field detuning.

Presenter: Lê Thị Ngọc Bảo

P.67 – Poster, NCTP-42

An A4 model with two Higgs singlets

Lam Hoang Thai, Do Thi Van Nhi, Nguyen Thanh Phong

Cantho University

We study the seesaw realization of a A4 model with two Higgs singlets. In this model, the mixing angle θ_{13} and leptogenesis are zero if the components of right handed neutrino mass matrix resulting from the two Higgs singlets are exact degenerate. We then study a tiny shift between aforementioned components. This minimal breaking results in deviations of lepton mixing angles from their tri-bimaximal mixing values in which the current experimental value of θ_{13} can be achieved. Besides, the baryon asymmetry of the Universe is successfully generated through non-zero leptogenesis by the decay of right handed neutrinos.

Presenter: Lam Hoang Thai

P.68 – Poster, NCTP-42

An application of q-deformed statistical method to lattice vibrations

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The deformed oscillators formalism plays a useful role in the study of physical models. Specifically, many variants of deformed oscillators have been used to study of the quantum optics, Condensed matter physics, etc... In this paper we consider the possibility for the application of the q-deformed statistical method to the problem in the theory of lattice vibrations. Our aim here is to construct a q-deformed crystal lattice vibration for generic atomic string, consider a statistical distribution in view of this vibration and calculate its thermodynamic potential.

Presenter: Hoàng Hạnh Phương

P.69 – Poster, NCTP-42

Linear and nonlinear optically detected electrophonon resonance in triangular quantum wells

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In this work, we study a detailed theory of linear and nonlinear optical absorption power in triangular quantum well (TrQW) when electrons are scattered with longitudinal optical phonons (LO phonons). The analytic expression for optical absorption power of electromagnetic waves caused by confined electrons is obtained in the case of electron-LO phonon scattering. Nonlinear optically detected electrophonon resonance (ODEPR) effect in a specific GaAs/AlGaAs quantum well with triangular potential is investigated. Conditions for the ODEPR are obtained based on the energy-momentum conservation law. From the curves expressing the dependence of the absorption power on photon energy we obtained the ODEPR-linewidths as profiles of the curves. Computational results show that the nonlinear ODEPR-linewidths increase with temperature and decrease with electric field amplitude.

Presenter: Pham Tuan Vinh

P.70 – Poster, NCTP-42

Effect of strain on electronic structure and thermoelectric property of a Bi2Te3/Sb2Te3 compound

Tran Van Quang, Nguyen Thi Hoa, Doan Thi Thuy Phuong*

Department of Physics, University of Transport and Communications, Hanoi, Vietnam

Compounds of bismuth telluride and antimony telluride have greatly attracted the attention of researchers in the years due to the potential applications in the fields of thermoelectrics and spintronics. In this work, we present first-principles calculation of a compound of bismuth telluride - antimony telluride using Quantum Espresso package within the framework of density functional theory. The results of electronic structure calculation show degenerate valleys at the band edges suggesting an enhancement of the power factor by band engineering. To substantiate, we use the solution of semi-classical Boltzmann's equation in a constant relaxation-time approximation to compute the transport coefficients, i.e. the Seebeck coefficient, the electrical conductivity, and the power factor. We demonstrate that the band topology near Fermi energy is tunable under the effects of strain which impacts efficiently on the transport property of the compound. The results suggest a promising technique to improve thermoelectric performance of the compound.

Presenter: Tran Van Quang

P.71 – Poster, NCTP-42

Excitonic condensation phase diagram in the extended Falicov-Kimball model with electron-phonon interaction

Do Thi Hong Hai (1,2,3) and Phan Van Nham (4)

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Influence of temperature on the excitonic condensation state in two-dimensional extended Falicov-Kimball model with electron-phonon interaction has been investigated by using the unrestricted Hartree-Fock approximation. Treating both the Coulomb interaction and the electron-phonon coupling in an equal footing, we analyze phase diagrams of the excitonic condensation state. At a given electron-phonon coupling, lowering temperature we find out a semimetal-excitonic condensate at a small Coulomb interaction and a semiconductor-excitonic condensate at a large Coulomb interaction. The excitonic condensate window is enlarged if the electron-phonon coupling is increased. A crossover from a BCS type to a BEC type of the excitonic condensation state driven either by the Coulomb interaction or the electron-phonon coupling in this systems at low temperature is also addressed.

Presenter: Do Thi Hong Hai

P.72 – Poster, NCTP-42

Production and decay of Higgs in the Randall-Sundrum model at high energy colliders

Bui Thi Ha Giang (1), Dao Thi Le Thuy (1), Dang Van Soa (2), Nguyen Thi Hau (3)

(1) Hanoi National University of Education; (2) Hanoi Metropolitan University; (3) Hanoi Uni-

versity of Mining and Geology

An attempt is made to present some experimental predictions of Higgs in the Randall-Sundrum model. We investigate the production of Higgs via e^+e^- and $\gamma\gamma$ colliders including the radion-Higgs mixing parameters. The production cross-sections in e^+e^- collisions are much larger than that in $\gamma\gamma$ collisions in the same conditions. The decay widths of Higgs depend strongly on the radion mass and the vacuum expectation value of the radion, so the existence of radion in the Randall-Sundrum model is necessary. The results also show that the dominant decay mode is $h \to b\bar{b}$.

Keywords: radion-Higgs mixing, decay widths, Randall-Sundrum model.

Presenter: Bui Thi Ha Giang

P.73 – Poster, NCTP-42

Controlling Band Gap of MoS2 Monolayer by Applying Pressure

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The MoS2 monolayer is a typical two-dimensional semiconductor of transition metal dichalcogenides, which have been attracting a great attention due to their promising potential for applications in nanotechnology. The existence of a band gap in the MoS2 monolayer is fascinating for applications in transistors fabrication. A control of the band gap of the MoS2 monolayer is a necessary engineering for developing nanoelectronics devices. Therefore, we studied the influence of pressure on MoS2 monolayer by using the density functional theory calculations. We analyzed the band structure and the electronic density of state of MoS2 before and after applying the pressure. We found that the width of the band gap of MoS2 monolayer strongly depends on pressure.

Presenter: Ong Kim Le

P.74 – Poster, NCTP-42

Computational predictions of the new Gallium nitride nanoporous structures

Le Thi Hong Lien, Do Thi Duong, Nguyen Thu Huyen and Vu Ngoc Tuoc

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

Nanoporous structural prediction is emerging area of research because of their advantages for a wide range of materials science and technology applications in opto-electronic, environment, sensors, shape-selective and bio-catalysis, to name just a few. We propose a computationally and technically feasible approach for predicting Gallium nitride nanoporous structures with hollows at the nano scale. The designed porous structures structures are studied with computations using the density functional tight binding and conventional density functional theory methods, revealing a variety of promising mechanical and electronic properties, which can potentially find future realistic applications. Their stability is discussed by means of the free energy computed within the lattice-dynamics approach. Our calculations also indicate that all the reported hollow structures are wide band gap semiconductors in the same fashion with their parent's bulk stable phase. The electronic band structures of these nanoporous structures are finally examined in detail.

Keyword: Gallium nitride, nanoporous; Structure prediction; Density functional tight-binding

Presenter: Le Thi Hong Lien

P.75 – Poster, NCTP-42

Investigation of Dark Matter in the $SU(3)_C \otimes SU(2)_L \otimes SU(3)_R \otimes U(1)_X$ model

Nguyen Tuan Duy (1), Le Duc Thien (2), Le Xuan Thuy (3), Do Thi Huong (1), Phung Van Dong (1)

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It is shown that the left-right asymmetric model based on $SU(3)_C \otimes SU(2)_L \otimes SU(3)_R \otimes U(1)_X$ gauge group, can provide dark matter naturally by the mean that dark matter candidates, their stable mechanism and relic density auto-matically arise from the gauge principles. We study the circumstance of dark matter corresponding to the electric charge parameter q=0. The packages mi-crOMEGAs is used to investigate the parameter spaces in the WMAP allowed region of the relic density. In addition, the indirect and direct searches for dark matter are also discussed.

Presenter: Le Duc Thien

P.76 – Poster, NCTP-42

Computational Analysis of Fish Behavior Responses in Chemical Stress Using Permutation Entropy and Fractal Dimension

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The movement behavior is an essential expression of life events of animals for survival (e.g., foraging, escaping).Various computational methods for analyzing motions of animals are outlined to address response behaviors of indicator animals under chemical stress.In this study, the Fractal Dimension (FD) and the Permutation Entropy (PE) were investigated to demonstrate behavioral changes before and after the treatments.The methodology was tested on 40 individuals of Zebrafish(Daniorerio), (20 control and 20 treatment fish (Diazinon, 1ppm) which was showed that FD and PE are variable before and after the treatment.The behavioral changes were accordingly obtained to reveal dynamic processes in continuous movement. FD and PE were promising tools for addressing structure property in response behavior of animals and could serve as an in situ monitoring tool to detect stressful agents in environment. Key words: Behavior monitoring,fractal dimension, permutation entropy, zebrafish, chemical stress.

Presenter: Quach Kha Quang

P.77 – Poster, NCTP-42

Study of Crystal-Amorphous Phase Transition and Morphologies of Metal Nanoparticle Fe under annealing

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Crystal-amorphous phase transition and morphologies of metal nanoparticles Fe (NPs) were investigated by means of molecular dynamics (MD) simulation. Calculations show that the amorphous NP is transformed into bcc crystal one when it was annealed for long times at 900K. According to simulation, at the early stage of the annealing, small nuclei form in different places of NP and dissolve for short times. After long times some nuclei form and gather nearby which create the stable clusters in the core of NP. After that, the crystal clusters grow in the direction to cover the core and then to spread into the surface of NP. The further study concerns different morphologies of Fe and FeB NPs. It was shown that different morphologies differ strongly not only in the core but also in the surface of NP. We found that the crystalline FeB NPs comprise a Fe crystal grain with defects and FeB amorphous phases. Comparing to the amorphous NP, the structural organization of phases in crystalline NPs is more complicated.

Keywords: molecular dynamics, crystal, amorphous, morphologies, phase transition.

Presenter: Pham Huu Kien

P.78 – Poster, NCTP-42

A study of non–extensive background fluctuation effect on a moving particle

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The contribution of extensive background fluctuations to effective mass of a moving particle in an environment has been investigated and has showed the dependence on only the characteristic parameters of background fluctuation such as rate parameter (λ) in Boltzmann, variance (α) in Gaussian and temperature (T) in back–body fluctuations. This field of interests is especially useful to provide physical insights of backgrounds. However, in the research of complex systems such as biological and ecological systems, it is not qualitatively adequate to model background fluctuations by a simple extensive distribution and to requires to take into account the non–extensiveness of the given background. In this work, an attempt to touch the non–extensiveness of an environment is analytically performed by using q–distributions and the dependence of effective mass on environmental non–extensive parameter is also discussed.

Presenter: Le Van Xuan

P.79 – Poster, NCTP-42

The size of the metal nanoparticle dependence of fluorescence resonance energy transfer

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We propose a model based on to understand fluorescence resonance energy transfer (FRET) between molecules (donor) and gold nanoparticle (acceptor). Mechanism of transferring energy from the electronically excited donors to acceptors is described in the spirit of a virtual photon

exchange. Additionally, the dipole-dipole interaction is supposed to dominate other forces in the electronic coupling. Our approach associated with experimental data shows that (1) conventional FRET is observed for small gold nanoparticle, and (2) FRET is found to be primarily due to surface energy transfer as increasing size of particles. This finding is in good agreement with previous studies and would pave the way for experimental investigation.

Presenter: Nguyen Minh Hoa

P.80 – Poster, NCTP-42

Simulation of diffusion barrier and osmotic diffusion for single component systems

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Barrier diffusion and osmotic diffusion are interesting diffusion processes. In the barrier diffusion, the diffusing flux vanishes although the concentration gradient is equal to zero and in the osmotic diffusion, although the concentration gradient is equal to zero, the diffusing flux does not vanish. The diffusion barrier and osmotic diffusion often occur in multi-component systems and their cause is coupled diffusion effect (the diffusing flux of a component is coupled strongly to its diffusing flux of partner). However, barrier diffusion and osmotic diffusion can occur in single component systems and its cause is the thermal velocity in the high concentration area is smaller than that the low concentration area. In this paper, on the random walk theory, the barrier diffusion and osmotic diffusion are simulated. The results show that: i) the barrier diffusion and osmotic diffusion can occur in single component system; ii) the cause of the barrier diffusion and osmotic diffusion is the difference of thermal velocity in areas together; iii) although the barrier diffusion and osmotic diffusion is contravariant to Fick's theory, they agree with the increasing entropy principle.

Presenter: Vu Ba Dung

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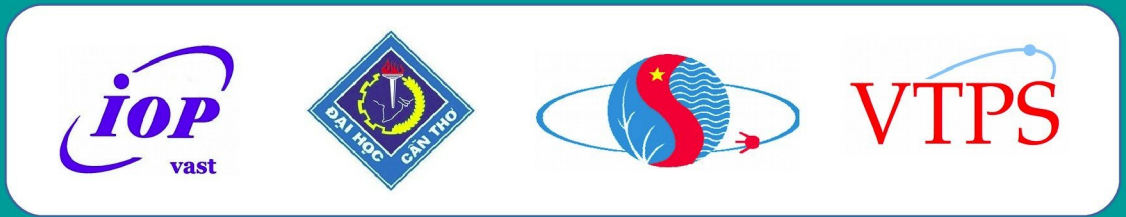
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