The 9th Asia-Pacific Workshop on Materials Physics

Hanoi, 12-15 December 2010

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Hanoi, 12-15 December 2010

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M. Mori (Sendai, Japan)

INVITED SPEAKERS

K. H. Ahn (Daejeon, Korea)
J. Akimtsu (Tokyo-Japan)
Y. Bang (Kwangju-Korea)
G. Baskaran (Chennai-India)
N. Bulut (Izmir-Turkey)
Wei-Qiang Chen (Hongkong)
P. C. Dai (Oak Ridge- USA)
X. Dai (Beijing-China)
H. T. Dung (Hochiminh City-Vietnam)
D. Feng (Fudan-China)
M. Fujita (Tohoku-Japan)

P. Fulde (APCTP-Germany)
T. Hanaguri (Riken-Japan)
N. V. Hieu (Hanoi City-Vietnam)
J. B. Hong (Seoul-Korea)
J. Ihm (Seoul-Korea)
C. Y. Kim (Seoul-Korea)
M. Kiselev (ICTP-Italia)
T.K. Lee (Taipei-Taiwan)
S. Maekawa (Tokai-Japan)
M. Micoulaut (Paris, France)
M. Mori (Tokai-Japan)
C. Y. Mou (Hsinchu-Taiwan)
N. Nagaosa (Tokyo-Japan)
G. Nogues (Grenoble CNRS-France)
Tai Kai Ng (Hongkong)
O. P. Sushkov (Sydney-Australia)
J. Tallon (Wellington-Newzealand)
T. Tohyama (Kyoto-Japan)
S. Uchida (Tokyo-Japan)
Y.J. Uemura (Columbia –USA)
N. L. Wang (Beijing-China)
T. Xiang (Beijing-China)
Xin-Cheng Xie (Beijing-China)
Jaejun Yu (Seoul-Korea)
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Institute of Physics (IOP, VAST)

Outline Program

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<tr><td>Time</td><td>Sun. 12 Dec.</td><td>Mon. 13 Dec.</td><td>Tue. 14 Dec.</td><td>Wed. 15 Dec.</td></tr>
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<tr><td>Lunch time</td><td colspan="3">Lunch: 12h25-14h00</td></tr>
<tr><td>Afternoon sessions:
14h00-18h00</td><td>Invited Talks
Poster session</td><td>Invited Talks</td><td rowspan="2">Free time, possible city tour</td></tr>
<tr><td>Evening</td><td>Reception for invited speakers:
18h00</td><td>Banquet:
18h00</td><td>Water Puppet theater:
20h00</td></tr>
</table>

Program Schedule

Time	Mon. 13/12	Tue. 14/12	Wed. 15/12
	Chair: Y. Bang	Chair: N. Bulut	Chair: M. Kiselev
09h00-09h25	**P. Fulde**	**N.V. Hieu**	**Lu Yu**
09h25-09h50	**J. Akimitsu**	**M. Fujita**	**D. Feng**
09h50-10h15	**S. Maekawa**	**J. Ihm**	**H.T. Dung**
10h15-10h45	**Coffee break** (30 min)		
	Chair: T. Tohyama	Chair: X. Dai	Chair: N.V. Hieu
10h45-11h10	**P. Dai**	**T.K. Lee**	**Jaejun Yu**
11h10-11h35	**N. Nagaosa**	**M. Mori**	**C.Y. Mou**
11h35-12h00	**N.L. Wang**	**O.P. Sushkov**	**M. Micoulaut**
12h00-12h25	**Y. Bang**	**S. Uchida**	**G. Baskaran**
12h25-14h00	**Lunch**		Closing (**N.V. Hieu**)
	Chair: T. Xiang	Chair: T.K. Ng	**Free time** **Possible city tour**
14h00–14h25	**C. Kim**	**J. Tallon**	
14h25-14h50	**T. Hanaguri**	**Y.J. Uemura**	
14h50-15h15	**T. Tohyama**	**W.Q. Chen**	
15h15-15h45	**Coffee-break** (30 min)		
	Chair: M. Mori	Chair: N.V. Lien	
15h45-16h10	**J.B. Hong**	**G. Nogues**	
16h10-16h35	**T.K. Ng**	**K.H. Ahn**	
16h35-17h00	**T. Xiang**	**M. Kiselev**	
17h00-17h25	**POSTER SESSION**	**X.C. Xie**	
17h25-18h00		(after 10 min break) **F. Pulizzi**	
Evening	**Banquet (from 18h00)**	**Water puppet theater (from 20h00)**	

The 9th Asia-Pacific Workshop on Materials Physics

SCIENTIFIC PROGRAM

December 13, 2010, Monday

08h00 – 08h30: Registration

08h30 - 09h00: Openings (P. Fulde, N.V. Hieu and S. Maekawa)

Chair: Y. Bang

09h00 - 09h25 **I - 1** **Non-phononic Interactions and Superconductivity**
P. Fulde
Asia Pacific Center for Theoretical Phyiscs, Pohang, Korea

09h25 - 09h50 **I - 2** **New superconductors recently developed by our group**
Jun Akimitsu
AOYAMA-GAKUIN University

09h50 - 10h15 **I - 3** **Spin Current, Charge Current and Heat Current in Magnetic Nanostructures**
Sadamichi Maekawa
Advanced Science Research Center, Japan Atomic Energy Agency, Tokai 319-1195, JapanJapan Science and Technology Agency, CREST, Tokyo 102-0075, Japan

Coffee Break (30')

Chair: T. Tohyama

10h45 - 11h10 **I - 4** **Electron-hole symmetry in the spin excitations of FeAs-based superconductors**
Pengcheng Dai
UT/ORNL/IOP

11h10 - 11h35 **I - 5** **Real-Time Dynamics of Correlated Electronic Systems**
Naoto Nagaosa
Dept. Applied Physics, The University of Tokyo

11h35 - 12h00 **I - 6** **Optical spectroscopy study on Fe-pnictides**
Nan Lin Wang
Institute of Physics, Chinese Academy of Sciences, Beijing, China

12h00 - 12h25 **I - 7** **Volovik effect in the +/-s-wave state for the iron-based superconductors**
Yunkyu Bang
Chonnam National University, Kwangju, Korea

Lunch

Chair: T. Xiang

14h00 - 14h25 **I - 8** **Photoemission studies of detwinned iron-pnictides: Band structures and Dirac cones**
Changyoung Kim
Insitute of Physics and Applied Physics, Yonsei University

14h25 - 14h50 **I - 9** **STM/STS studies on iron-based superconductors**
Tetsuo Hanaguri
Magnetic Materials Laboratory, RIKEN Advanced Science Institute, 2-1 Hirosawa, Wako, Saitama 351-0198, JAPAN

14h50 - 15h15 **I - 10** **Electronic and Magnetic Properties in the Antiferromagnetic Metallic Phase of Iron Pnictide Superconductors**
Takami Tohyama
Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan

Coffee Break (30')

Chair: M. Mori

15h45 - 16h10 **I - 11** **Quasiparticle tunneling in a nanocontact system under bias**
Jongbae Hong
Department of Physics and Astronomy, Seoul National University

16h10 - 16h35 **I - 12** **Topological order in Classical Systems**
Tai Kai Ng
Hong Kong University of Science and Technology, Hong Kong

16h35 - 17h00 **I - 13** **Optimizing Hartree-Fock orbitals by the density-matrix renormalization group**
H.-G. Luo, M.-P. Qin, T. Xiang
Institute of Physics, Chinese Academy of Sciences
Institute of Theoretical Physics, Chinese Academy of Sciences

Chair: N.H. Quang

17h00 - 18h00 **P - 1** **Influence of Phonon Confinement on Absorption Influence of Phonon Confinement on Absorption Power and Line-Widths in Rectangular Quantum Wires**
Le Dinh, Le Quoc Anh and Tran Cong Phong
Department of Physics, Hue University's College of Education 32 Le Loi, Hue, Vietnam

P - 2 **First-principles investigations of the dielectric properties of Silicon Nitride films**
T. Anh Pham (1), Tianshu Li (1), Francois Gygi (2,3) and Giulia Galli (1,4)
(1) Department of Chemistry, University of California Davis
(2) Department of Applied Science, University of California Davis
(3) Department of Computer Science, University of California Davis
(4) Department of Physics, University of California Davis

P - 3 **Light Absorption by excitons in bilayer parabolic quantum dots**

Nguyen Hong Quang and Nguyen Duong Bo
Institute of Physics, VAST, 10 Dao Tan, Ba Dinh, Hanoi, Vietnam

P - 4 **Dirac electrons under a tunable potential barrier in graphene.**

Tran Nguyen Dung, Nguyen Hai Chau
Institute of Physics, VAST

P - 5 **Mechanism of Solidification of Vitreous GeO_2 Nanoparticles**

Tran Phuoc Duy, Vo Van Hoang
Department of Physics, Institude of Technology, HoChiMinh city National University 268 Ly Thuong Kiet Street, District 10, HoChiMinh City-Vietnam

P - 6 **Structural properties of simulated liquid GaxAsy**

Tran Thi Thu Hanh, Vo Van Hoang
Department of Applied physics, Institute of Technology National University of Hochiminh City 268 Ly Thuong Kiet Str., Distr. 10, Hochiminh City, Vietnam

P - 7 **Calculations of pressure dependence of EXAFS cumulants in zinc-blende semiconductors**

Ho Khac Hieu (1) and Vu Van Hung (2)
(1) National University of Civil Engineering, 55 Giai Phong, Hai Ba Trung, Hanoi, Vietnam
(2) Hanoi National University of Education, 134 Xuan Thuy, Cau Giay, Hanoi, Vietnam

P - 8 **Optical sum frequency microscopy of cellulose fibers**

Hoang Chi Hieu (1), Nguyen Anh Tuan (1,2), Hongyan Li (1,2), Goro Mizutani (1,2)
(1) School of Materials Science, Japan Advanced Institute of Science and Technology 1-1 Asahidai Nomi, Ishikawa 923-1292, Japan
(2) Japan Science and Technology Agency, Core Research for Evolutional Science and Technology, 5-3 Sanban-cho, Chiyoda-ku, Tokyo 102-0075, Japan

P - 9 **Photocatalytic activity of transition-doped TiO2-d nanobelts synthesized by metalorganic chemical vapor deposition**

Nguyen Thi Quynh Hoa (1), Eui-Tae Kim (2)
(1) Department of Technology, Vinh University, 182 Le Duan, Vinh, Vietnam
(2) Department of Materials Science and Engineering, Chungnam National University, Daeduk Science Town, Daejeon 305-764, Korea

P - 10 **Preparation of Water-soluble Multi-walled Carbon Nanotubes Using Simple Oxidizing Agent**

Nguyen Ngoc Hoang, Jarrn-Horng Lin
National university of Tainan, Department of Materials science, Tainan 70005, Taiwan

P - 11 **The Nonlinear Electrical Conduction in Parabolic Quantum Wells**

Tran Cong Phong (1), Bui Dinh Hoi (2)
(1) Hue University's College of Education, 32 Le Loi Str., Hue City, Viet Nam;
(2) National University of Civil Engineering, 55 Giai Phong Str., Hai Ba Trung, Ha Noi, Viet Nam

P - 12 **Spin dependent transport in ferromagnetic gate graphene structures**

V. Hung Nguyen (1,2), V. Nam Do (3), A. Bournel (1), P. Dollfus (1)
(1) Institut d'Electronique Fondamentale, UMR8622, CNRS, Univ. Paris Sud, 91405 Orsay, France.
(2) Center for Computational Physics, Institute of Physics, VAST, PO Box 429 Bo Ho, Hanoi 10000, Vietnam.
(3) Hanoi Advanced School of Science and Technology, 40 Ta Quang Buu, Hanoi 10000, Vietnam.

P - 13 **Study on the formation of nano-structure for TiO2 material**

Ngo Thu Huong, Do Thi Kim Anh and Hoang Nam Nhat
Vietnam National University, Hanoi 144 Xuan Thuy, Cau Giay, Hanoi, Vietnam

P - 14 Photoluminescence of ZnO nanocolloid

Ngo Thu Huong, Dinh Thi Lan, Vu Thi Phuong Thanh, Hoang Nam Nhat
Vietnam National University Hanoi, 144 Xuan Thuy, Cau Giay, Ha Noi, Viet Nam

P - 15 Synthesize and research Au coated APTES/SiO2/Fe3O4 nanoparticles by seed-mediated method, potentially application in biomedicine.

Truong Thuy Kieu (1), Tran Hoang Hai (1), Tran Thi Khanh Chi (2), Do Minh Duc (3), Le Hong Phuc (1), Le Khanh Vinh (1), Bui Duc Long (1), Nguyen Quan Hien (1), and Duong Ai Di (3)
(1) Ho Chi Minh City Institute of Physics.
(2) College of Technology
(3) Can Tho University.

P - 16 Novel simulations on chain-like formation of ferrofluids: influence of anisotropy.

Tran Nguyen Lan and Tran Hoang Hai
HoChiMinh City Institute of Physics, Vietnamese Academic of Science and Technology, Vietnam

P - 17 Nanoscale crystalline nucleation of supercooled liquid gold

Truong Nguyen Duy Ly, Vo Van Hoang
Department of Physics, Institute of Technology , HoChiMinh City National University 268 Ly Thuong Kiet Street, District 10, HoChiMinh City, Viet Nam.

P - 18 Investigation of the Glass-to-Liquid Process of Monatomic Lennard-Jones glass

Le Nguyen Tue Minh, Vo Van Hoang
Department of Physics, Institude of Technology of HochiMinh City, 268 Ly Thuong Kiet Street, District 10, HoChiMinh City-Vietnam

P - 19 High TC phase transition in Li-doped Bi-2223 thin films grown by pulse laser deposition method

N T Mua (1,2), T D Hien (2) and N K Man (2)
(1) Hanoi University of Prevention and Fight Fire, No. 243 Khuat Duy Tien, Thanh Xuan, Hanoi, Vietnam

(2) International Training Institute for Materials Science (ITIMS), Hanoi University of Technology, No. 1, Dai Co Viet Road, Hanoi, Vietnam

P - 20 Computer Simulation of the Diffusion Processes in one-Dimensional Disordered Systems

T. V. Mung, P. K. Hung, P. N. Nguyen. N.V.Hong
Department of Computational Physics, Hanoi University of Technology, Vietnam - 1 Dai Co Viet, Hanoi Viet Nam

P - 21 Optically detected electrophonon resonance effects in compositional semiconductor superlattices

Tran Cong Phong (1), Luong Van Tung (2), Vo Thanh Lam (3)
(1) Department of Physics, Hue University's College of Education 32 Le Loi, Hue,Vietnam
(2) Department of Physics, Dong Thap University 783 Pham Huu Lau, Cao Lanh, Dong Thap, Viet Nam
(3) Department of Natural Sciences, Sai Gon University 273 An Duong Vuong, District 5, Ho Chi Minh, Viet Nam

P - 22 Calculation of Temperature Dependence of Absorption Line-Widths in Cylindrical Quantum Wires

Huynh Vinh Phuc (1), Tran Cong Phong (2)
(1) Department of Physics, Dong Thap University, Cao Lanh, Vietnam (2) Department of Physics, Hue University's College of Education, Hue, Vietnam

P - 23 A Theory of Linewidth for Nonlinear Optical Conductivity in Rectangular Quantum Wires

(1) Tran Cong Phong, (2) Huynh Vinh Phuc
(1) Department of Physics, Hue University's College of Education 32 Le Loi, Hue, Viet Nam
(2) Department of Physics, Dong Thap University, 783 Pham Huu Lau, Cao Lanh, Dong Thap, Viet Nam

P - 24 Optically Detected Electron Energy Spectrum in Cylindrical Quantum Wires

Tran Cong Phong (1), Le Thi Thu Phuong (1)
(1) Hue University's College of Education, 32 Le Loi, Hue, Viet Nam

P - 25 Rate of phonon excitation and conditions for phonon generation in rectangular quantum wires

Le Thi Thu Phuong (1), Tran Cong Phong (1)
(1) Hue University's College of Education, 32 Le Loi, Hue, Viet Nam;

P - 26 White Light Emission from Nano-structured Materials

Nguyen Hong Quang (1), Luu Tien Hung (1), and Nguyen Thi Quynh Hoa (2)
(1) Department of Physics, Vinh University, 182 Le Duan Street, Vinh City, VIETNAM
(2) Department of Technology, Vinh University, 182 Le Duan Street, Vinh City, VIETNAM

P - 27 Investigation of Optical Response in Antiferromagnetic Phase of Iron Pnictides with Mean-Field Approximation

Koudai Sugimoto (1), Eiji Kaneshita (2), Takami Tohyama (1,3)
(1) Yukawa Institute for Theoretical Physics, Kyoto University;
(2) Sendai National College of Technology
(3) JST-TRIP

P - 28 Properties of Polypyrrole and Single Wall Carbon Nanotubes Composites

Le Hai Thanh, Nguyen Trong Tung, Nguyen Duc Thien and Duong Ngoc Huyen
Institute of Engineering Physics Hanoi University of Science and Technology

P - 29 Structure and Properties of $Ca_{0.85}Pr_{0.15}Mn_{1-y}Ru_yO_3$ (y = 0-0.2) Thin Films Fabricated by PLD Technique

Phung Quoc Thanh, Seong-Cho Yu, Nguyen Duc Tho, and Hoang Nam Nhat
Vietnam National University Hanoi, 144 Xuan Thuy, Cau Giay, Hanoi, Vietnam

P - 30 Efficient 3D Poisson solvers using post-BICGSTAB algorithms

Dinh Nhu Thao

Hue University of Pedagogy, 34 Le-Loi Street, Hue City, Vietnam

P - 31 Electronic structure of a molecular magnet from salicylate based copper complex

Nguyen Duc Tho, Hoang Duc Anh, Phung Quoc Thanh and Hoang Nam Nhat
Vietnam National University, Hanoi 144 Xuan Thuy, Cau Giay, Hanoi, Vietnam

P - 32 Orange photoluminescence of nanosize materials based ZnS

Nguyen Minh Thuy, Tran Minh Thi and Nguyen thi Van Anh
Department of Physics, Hanoi National University of Education

P - 33 Electronic Structure of EU- DOPED CaO by Density Functional Theory

Nguyen Thuy Trang (1) and Hoang Nam Nhat (2)
(1) Laboratory for Computational Materials Science, Hanoi University of Sciences, Vietnam National University Hanoi, 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam
(2) Faculty of Technical Physics and Nanotechnology, University of Engineering and Technology, Vietnam National University Hanoi, 144 Xuan Thuy, Cau Giay, Hanoi, Vietnam

P - 34 Transparent thin film nanostructure device

Uday Trivedi (1) and Utpal Joshi (2)
(1)Government Engineering College,Chandkheda 382424,Ahmedabad-India.
(2) Gujarat University-380015, Ahmedabad-India

P - 35 Coherent potential approximation study of transport properties in the ionic Hubbard model on half-filled bipartite lattice

Hoang Anh Tuan and Nguyen Tri Lan
Institute of Physics, VAST POBox 429, BoHo, Hanoi 10 000

P - 36 Spin orbit coupling in graphene nano-ribbons
C. Huy Pham, H. Chau Nguyen, L. Tung Nguyen
Institute of Physics, Vietnam

P - 37 Investigation local physic-mechanical properties of thin polymer layers using Atomic Force Microscopy
Nguyen Hoang Yen(1), Vo Thanh Tung(1), Nguyen Trong Tinh(2), S.A. Chizhik(3)
(1) Physics department, Hue College of Sciences, Hue University, 77 Nguyen Hue str., Hue city, Vietnam
(2) Institute of Applied Physics and Scientific Instrument, Vietnamese Academy of Science and Technology, 18 Hoang Quoc Viet , Cau giay, Hanoi Vietnam
(3) National Academy of Sciences of Belarus, Minsk, Belarus

P - 38 Long range disorder effects on the heat capacity of two dimensional electron systems
Cristine Villagonzalo (1) and Rayda P. Gammag (1)
(1) Structure and Dynamics Group, National Institute of Physics University of the Philippines, Diliman, Quezon City 1101, Philippines

P - 39 Deposition of SnO_2 and SnO_2:F thin films by pneumatic sprayer deposition and study their optical and electrical properties
Pham Van Vinh, Nguyen Van Hung, Nguyen Thi Dung
Hanoi National University of Education

P - 40 Ethanol gas sensor based on SnO_2/ZnO and ZnO:Al films deposited by pneumatic sprayer deposition
Pham Van Vinh, Nguyen Van Hung , Bui Thi Hai and Dao Thi Hong Le
Hanoi National University of Education

P - 41 DFT Study of Raman scattering in Fe-doped $CaMnO_3$
Pham Duc Huyen Yen, Hoang Nam Nhat
Vietnam National Univbersity Hanoi 144 Xuan Thuy, Cau Giay, Hanoi, Vietnam

P - 42 **The Electronic Properties of MgO under High Pressure from Ab Initio Calculations**

G. Zheng (1,2), L. Yu (1,2), K.H. He (1,2)
(1) School of Mathematics and Physics, China University of Geosciences, Wuhan, 430074, China
(2) Institute of Material Modeling and Computational Physics, China University of Geosciences, Wuhan, 430074, China

Banquet (From 18h00)

December 14, 2010, Tuesday

Chair: N. Bulut

09h00 - 09h25 **I - 14** **Engineered Spin Chains for Perfect Quantum State Transfer**

Nguyen Van Hieu
Institute of Materials Science, VAST, Hanoi, Vietnam

09h25 - 09h50 **I - 15** **Neutron-scattering study of novel spin correlations in high-Tc superconductors**

Masaki Fujita (1), Masanori Enoki (2), Satoshi Iikubo (3), Kazuyoshi Yamada (4)
(1) Institute for Materials Research, Tohoku University
(2) Department of Physics, Tohoku University
(3) Graduate School of Life Science and Systems Engineering, Kyushu Institute of Technology
(4) World-Premier-International Research Center Initiative, Tohoku University

09h50 - 10h15 **I - 16** **Vortex current and induced magnetic fields originated from defects in metallic carbon nanotubes**

Jisoon Ihm
Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea

Coffee Break (30')

Chair: X. Dai

10h45 - 11h10 I - 17 **Anomalous collective excitations of cuprates**
Chung-Pin Chou and T. K. Lee
Institute of Physics, Academia Sinica, Taipei, Taiwan

11h10 - 11h35 I - 18 **Possible mechanisms of enhanced pairing gap near apical and dopant oxygens in cuprate**
Mori M (1,2), Khaliullin G (3), Tohyama T (4), Maekawa S (1,2)
(1) Japan Atomic Energy Agency;
(2) JST-CREST;
(3) Max Planck Institute;
(4) Kyoto University

11h35 - 12h00 I - 19 **Effective action, magnetic excitations and quantum fluctuations in lightly doped single layer cuprates**
Oleg P. Sushkov
University of New South Wales

12h00 - 12h25 I - 20 **Electronic Anisotropy in Cuprates and Fe-Arsenides**
Shin-ichi Uchida (1,2)
(1) Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033, Japan
(2) JST, Transformative Research-Project on Iron Pnictides, Tokyo 102-0075, Japan

Lunch

Chair: T. K. Ng

14h00 - 14h25 I - 21 **Pairing fluctuations and quantum critical fluctuations in HTS cuprates**
Jeffery Tallon
MacDiarmid Institute for Advanced Materials and Nanotechnology, and Industrial Research Ltd

14h25 - 14h50 I - 22 **Common behaviors of unconventional superconductors indicating non-BCS condensation and spin-mediated resonant pairing**
Yasutomo J. Uemura
Physics Department, Columbia University, New York, USA

14h50 - 15h15 **I - 23** **Possible π-junction in iron pnictide superconductors with antiphase s-wave pairing**

Wei-Qiang Chen(1), Fengjie Ma(2,3), Zhong-Yi Lu(2), and Fu-Chun Zhang(1)
(1) Department of Physics, and Center of Theoretical and Computational Physics, the University of Hong Kong, Hong Kong, China;
(2) Department of Physics, Renmin University of China, Beijing 100872, China;
(3) Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China

Coffee Break (30')

Chair: N. V. Lien

15h45 - 16h10 **I - 24** **Studying the properties of superconductors with ultracold atoms**

Gilles Nogues
Institut Néel, CNRS and Laboratoire Kastler Brossel, Ecole Normale Supérieure

16h10 - 16h35 **I - 25** **0.7 conductance anomaly: Multiple existence of Kondo impurities in a quantum point contact**

Kang-Hun Ahn
Department of Physics, University of Bath, UK

16h35 - 17h00 **I - 26** **Thermoelectric transport through a quantum dot: Interplay between FL and NFL behavior**

M.N.Kiselev, V.E. Kravtsov and T.K.T. Nguyen
ICTP, Strada Costiera 11, I-34151 Trieste, Italy

17h00 - 17h25 **I - 27** **Dephasing, disorder and interaction effects in 2D topological insulator**

Xincheng Xie
Peking University and Institute of Physics, Chinese Academy of Sciences

Break 10'

17h35 - 18h00 **I - 28** **F. Pulizzi**

Water puppet theater (From 20h00)

December 15, 2010, Wednesday

Chair: M. Kiselev

09h00 - 09h25 I - 29 **Non-BCS superconductivity for underdoped cuprates by spin-vortex attraction**

Lu Yu
Institute of Physics, Chinese Academy of Sciences

09h25 - 09h50 I - 30 **Orbital characters of iron-based superconductors and their parent compounds**

Y. Zhang (1), L. X. Yang (1), F. Chen (1), C. He (1), X. H. Chen (2), M. Arita (3), K. Shimada (3), H. Namatame (3), M.Taniguchi (3), D. L. Feng (1)
(1) Department of Physics, State Key Laboratory of Surface Physics, and Advanced Material Laboratory, Fudan University, Shanghai 200433, P. R. China
(2) Department of Physics, University of science and technology of China, Hefei 230027, P. R. China
(3) Hiroshima Synchrotron Radiation Center, Hiroshima University, Hiroshima 739-8526, Japan.

09h50 - 10h15 I - 31 **Quantum-ensured comparative voting and anonymous broadcast channels**

Ho Trung Dung (1), Mark Hillery (2)
(1) Institute of Physics, Academy of Sciences and Technology 1 Mac Dinh Chi Street, District 1, Ho Chi Minh City, Vietnam
(2) Department of Physics, Hunter College of CUNY, 695 Park Avenue, New York, NY 10065, USA

Coffee Break (30')

Chair: N. V. Hieu

10h45 - 11h10 **I - 32** **Novel Spin-Orbit Physics in 5d Transition Metal Oxides**

Jaejun Yu

Center for Strongly Correlated Materials Research Department of Physics and Astronomy Seoul National University Seoul 151-747, Korea

11h10 - 11h35 **I - 33** **Density of states of graphene in the presence of strong point defects**

Chung-Yu Mou

Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

11h35 - 12h00 **I - 34** **Rigidity in amorphous networks: from simple sulphides to complex phase-change tellurides**

M. Micoulaut

LPTMC, Université Pierre et Marie Curie, Boite 121 4, place Jussieu, 75252 Paris cedex 05 France

12h00 - 12h25 **I - 35** **Anderson-Haldane Liquid: a novel Resonating Valence Bond Metallic State**

G. Baskaran

The Institute of Mathematical Sciences Chennai 600 113, India

Closing (N. V. Hieu)

The Asia-Pacific Workshop on Materials Physics

Hanoi, 12-15 December 2010

ABSTRACTS

1. Non-phononic Interactions and Superconductivity

P. Fulde

Asia Pacific Center for Theoretical Phyiscs, Pohang, Korea

We want to discuss two cases, where there is unambiguous experimental evidence that non-phononic interactions cause Cooper pairing. One is the filled skutterudite PrOs4Sb12. Here intra-atomic excitations within the 4f shell couple to conduction electrons and cause a doubling of Tc as compared with LaOs4Sb12. The second example is UPd2Al3 where magnetic excitations provide the glue for Cooper pair formation.

2. New superconductors recently developed by our group

Jun Akimitsu

AOYAMA-GAKUIN University

In this conference, we review the new superconductors or possible new superconductor recently developed by our group. We present here, (I) Superconductivity in the carrier-doped wide gap semiconductors. (II-1) Tm-based reentrant superconductor Tm5Rh6Sn18. (II-2) Highly anisotropic gap functions in a non-magnetic superconductor Y5Rh6Sn18. (â…¢) Spin-orbit Mott insulating antiferromagnet Ba2IrO4 and its carrier doping.

3. Spin Current, Charge Current and Heat Current in Magnetic Nanostructures

Sadamichi Maekawa

Advanced Science Research Center, Japan Atomic Energy Agency, Tokai 319-1195, and Japan Science and Technology Agency, CREST, Tokyo 102-0075, Japan

In magnetic nanostructures, there are two conservation laws between the conduction electrons and the magnetic moment. The first is the angular momentum conservation which brings about the spin angular momentum transfer between them. This is a key concept for controlling the magnetization direction in a variety of spintronic devices. The other is that of energy stored in the conduction electrons and the magnetic moment. The magnetic energy stored in the conduction electrons is released as the spin motive force. The spin-motive force is derived by extending the Faraday's law of electro-magnetism. The non- conservative force acting on the spins of conduction electrons causes the work, which brings about the spin-motive force. A variety of the phenomena and the application in magnetic nanostructures [1] are presented and discussed based on the conservation laws.

[1] Concept in Spin Electronics, ed. S. Maekawa (Oxford University Press, 2006).

4. Electron-hole symmetry in the spin excitations of FeAs-based superconductors

Pengcheng Dai

UT/ORNL/IOP

In this talk, I will present our most recent neutron scattering studies of electron-hole symmetry in the spin excitations of FeAs-based superconductors. It is well known that the parent compounds of FeAs-based superconductors are antiferromagnetic and superconductivity in these materials arise from suppression of the static antiferromagnetic order. We use inelastic neutron scattering to systematically investigate the spin excitations in both electron and hole-doped materials. While both electron and hole-doped materials have a neutron spin resonance,

the detailed temperature and wavevector dependene of the spin excitations are quite different. We discuss their relevance to superconductivity.

5. Orbital characters of iron-based superconductors and their parent compounds

Y. Zhang (1), L. X. Yang (1), F. Chen (1), C. He1, X. H. Chen (2), M. Arita (3), K. Shimada (3), H. Namatame (3), M.Taniguchi (3), D. L. Feng (1)

(1) Department of Physics, State Key Laboratory of Surface Physics, and Advanced Material Laboratory, Fudan University, Shanghai 200433, P. R. China

(2) Department of Physics, University of science and technology of China, Hefei 230027, P. R. China

(3) Hiroshima Synchrotron Radiation Center, Hiroshima University, Hiroshima 739-8526, Japan.

Multiple degrees of freedom play important roles in the physics of iron-based high-temperature superconductors (Fe-HTSC) and their parent compounds. For example, there is a magnetically ordered spin density wave phase in the vicinity of the superconducting phase, while the spin density wave transition is ubiquitously accompanied by a structural transition in various families of iron-based systems. The orbital degree of freedom is an important factor in iron-based superconductors. For example, possible orbital ordering has been associated with the spin density wave, and we recently found that the superconducting gap sizes are different at the same Fermi momentum for two bands with different spatial symmetries (one odd, one even). In the talk, I will present our recent angle resolved photoemission spectroscopy (ARPES) data on the electronic structure of various iron pnictides. We studied the orbital characters of the electronic structure in optimally electron-doped $BaFe_{1.85}Co_{0.15}As_2$ by exploiting the detailed polarization-sensitivity of the orbitals in ARPES. We observe strong polarization dependence of all the bands near Fermi energy, and conducted systematic analysis. The orbital characters of the low energy electronic structure and Fermi surface in three dimensional momentum space are determined. Our results indicate that the

previous orbital assignments of band structure calculations are just partially correct. Particularly, the contributions of the dxy and dx2-y2 orbitals were not right. Our results lay the foundation for constructing realistic microscopic models of iron-based superconductors. Furthermore, we studied the transport properties and electronic structure of magnetically detwinned NaFeAs, and AEFe2As2. We identify the roles of various orbitals in the spin density wave formation.

6. Optical spectroscopy study on Fe-pnictides

Nan Lin Wang

Institute of Physics, Chinese Academy of Sciences, Beijing, China

The interplay between the superconductivity and magnetism has attracted much attention in the field of Fe-based superconductors. To shed light on the origin of the magnetism in the compounds we investigated the charge excitations and dynamics of Fe-based materials by optical spectroscopy measurements. For all FeAs-based parent compounds we observed common spectral features for E//ab-plane: partial energy-gaps formation leading to a removal of a large part of free-carrier spectral weight and a steep reduction of the carrier scattering rate in the magnetic ordered state. However, the 11-type FeTe behaves very differently. No energy gap opens in the magnetic state. We suggest that both the itinerancy and local moment interactions of Fe 3d electrons are present in the systems, but they contribute differently to the magnetic instabilities in different systems. I shall also present the c-axis polarized measurements on the parent and doped superconducting compounds of 122-based systems, and elaborate their significant difference from the E//ab-plane. The different optical responses between E//ab-plane and E//c-axis were explained by invoking the different Fermi surface topologies of the materials. Work done with Z. G. Chen, W. Z. Hu, G. Li, J. Dong, T. Dong, R. H. Yang, B. F. Hu, B. Cheng, P. Zheng, G. F. Chen, J. L. Luo, Z. Fang, and X. Dai.

7. Volo1vik effect in the +/-s-wave state for the iron-based superconductors

Yunkyu Bang

Chonnam National University, Kwangju, Korea

We studied the field dependencies of specific heat coefficient $\gamma(H) = C(T,H)/T$ and thermal conductivity coefficient $\kappa(T,H)/T$ of the s-wave state in the mixed state [1]. We found that it is a generic feature of the two band s-wave state with the unequal sizes of gaps, small S and large L, that Doppler shift of the quasiparticle excitations (Volovik effect) creates a finite density of states, on the extended states outside of vortex cores, proportional to H in contrast to the -H dependence of the d-wave state. Impurity scattering effect on the s-wave state, however, makes this generic H-linear dependence sublinear approaching to the H behavior. Our calculations of $\kappa(T,H)/T$ successfully fit the experimental data of $Ba(Fe_{1-x}Co_x)2As_2$ with different Co-doping x by systematically varying the gap size ratio $R= |S| / |L|$. We also resolve the dilemma of a substantial value of $\gamma(H) = C(T,H)/T$ but almost zero value of $\kappa(T,H)/T$, as observed in experiments [2].

[1] Yunkyu Bang et al, Phys. Rev. Lett. 104, 217001 (2010).

[2] M.A. Tanatar et al, Phys. Rev. Lett. 104, 067002 (2010).

8. Photoemission studies of detwinned iron-pnictides: Band structures and Dirac cones

Changyoung Kim

Insitute of Physics and Applied Physics, Yonsei University

We performed angle resolved photoelectron spectroscopy (ARPES) studies on mechanically detwinned $BaFe_2As_2$. We observe distinct band dispersions along the two crystal axes Gamma-X and Gamma-Y, indicating detwinning of the magnetic domains. The shapes and characters of the Fermi surfaces are identified. Shapes of the two hole pockets around the Gamma- point are found to be consistent with the Fermi surface topology predicted in the orbital ordered states. Near the Gamma-point, Dirac-cone like band dispersions are clearly

identified as theoretically predicted. The observed band dispersions are compared with calculated band structures. With a magnetic moment of 0.2 mu_B per iron atom, there is a good agreement between the calculation and experiment. We also find the electronic structure very sensitive to the As height.

9. STM/STS studies on iron-based superconductors

Tetsuo Hanaguri

Magnetic Materials Laboratory, RIKEN Advanced Science Institute, 2-1 Hirosawa, Wako, Saitama 351-0198, JAPAN

Scanning tunneling microscopy/spectroscopy (STM/STS) has proven to be a powerful technique to elucidate the electronic states of unconventional superconductors. We have applied STM/STS to investigate the superconducting gap of iron-based superconductors. We discuss magnetic-field effect on the interference patterns of Bogoliubov quasi-particles in Fe(Se.Te), which indicates that the superconducting gap possesses s+- structure. We also argue the tunneling spectra at the defects in LiFeAs in relation to the symmetry of the gap.

10. Electronic and Magnetic Properties in the Antiferromagnetic Metallic Phase of Iron Pnictide Superconductors

Takami Tohyama

Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan

We examine electronic states and magnetic properties of antiferromagnetic (AF) metallic phase in iron pnictides by mean-field and RPA calculations. We find that a five-band model exhibiting a small magnetic moment, inconsistent with the first-principles calculations, reproduces well not only gap magnitude but also anisotropic spectral weight in the optical conductivity [1,2]. Collective and continuum excitations in the spin channel are investigated by RPA calculations for the five-band model for both the AF and paramagnetic phases. We found that the particle-hole gap opening in the bare susceptibility is crucial to obtain spin excitations fully consistent with inelastic neutron scattering data [3]. Furthermore, we investigate Dirac

fermions in the AF metallic phase. Deriving an effective Hamiltonian for the Dirac fermions, we reveal that there exist two Dirac cones carrying the same chirality, contrary to graphene, compensated by a Fermi surface with a quadratic energy dispersion as a consequence of a non-trivial topological property inherent in the band structure. The presence of the Dirac fermions gives the difference of sign-change temperatures between the Hall coefficient and the thermopower, being consistent with available experimental data [4].

[1] E. Kaneshita, T. Morinari, and T. Tohyama, Phys. Rev. Lett. 103, 247202 (2009).

[2] K. Sugimoto, E. Kaneshita and T. Tohyama, in preparation.

[3] E. Kaneshita and T. Tohyama, to be published in Phys. Rev. B; arXiv:1002.2701.

[4] T. Morinari, E. Kaneshita, and T. Tohyama, Phys. Rev. Lett. 105, 037203 (2010).

11. Quasiparticle tunneling in a nanocontact system under bias

Jongbae Hong

Department of Physics and Astronomy, Seoul National University

In recent experimental studies on a nanocontact system under bias, various dI/dV lineshapes, where I and V denote the current and the bias, are reported. However, such lineshapes are explained via the single-particle point of view. In particular, theoretical dI/dV lineshapes that fit experiments have not been obtained. In this talk, we present the dI/dV lineshapes constructed by quasiparticle tunneling that considers many-body coherent effect. We show that two resonant tunneling levels are formed near the Fermi level when the nanocontact system has two electron reservoirs. Under bias, unidirectional quasiparticle tunneling occurs through these levels and the dI/dV lineshape has peaks or shoulders. The quasiparticle tunneling through the resonant tunneling levels formed by two electron reservoirs may explain the dI/dV lineshapes observed by scanning tunneling spectroscopy and those given in a quantum point contact. We employ the single-impurity Anderson model with two reservoirs as a model of nanocontact system and calculate the retarded Green's function that contains the effect of bias

12. Topological order in Classical Systems

Tai Kai Ng

Hong Kong University of Science and Technology, Hong Kong

In this talk I shall give a general introduction to the idea/origin of topological order in classical systems. Two classical Ising-like models will be discussed as examples of classical topological order. The relation to quantum topological order will be discussed.

13. Optimizing Hartree-Fock orbitals by the density-matrix renormalization group

H.-G. Luo, M.-P. Qin, T. Xiang

Institute of Physics, Chinese Academy of Sciences Institute of Theoretical Physics, Chinese Academy of Sciences

We have proposed a density-matrix renormalization group (DMRG) scheme to optimize the one-electron basis states of molecules. It improves significantly the accuracy and efficiency of the DMRG in the study of quantum chemistry or other many-fermion system with nonlocal interactions. For a water molecule, we find that the ground state energy obtained by the DMRG with only 61 optimized orbitals already reaches the accuracy of best quantum Monte Carlo calculation with 92 orbitals.

14. Engineered Spin Chains for Perfect Quantum State Transfer

Nguyen Van Hieu

Institute of Materials Science, VAST, Hanoi, Vietnam

For the application to the quantum information processing technology the quantum state transfer (QST) between two directly interacting qubits as well as between two distant ones interacting through the intermediary of different quantum systems were widely considered. As the intermediary system it was proposed to use that of photons in an optical fiber for the case of the QST between two quantum dots placed inside two microcavities connected through this optical fiber [1-4], or a network of interacting spins in the case of the QST between two spin-qubits interacting with this network [5-10]. It is known that the perfect QST from one end of a homogeneous N-qubit chain to

another is possible only for N = 2 and 3. In order to achieve the perfect QST it was proposed to use engineered spin chains with untunable but modulated coupling between adjacent spins, and a special version of engineered spin chains allowing the perfect QST was found in literature. The purpose of this work is to establish a wide class of engineered inhomogeneous mirror-symmetric N-spin chains with modulated untunable couplings which can provide the perfect QST between two ends of each chain. It includes as special cases the spin chains previously proposed. The sufficient conditions for the engineered mirror-symmetric spin chains allowing the perfect QST are derived. From these conditions the algebraic equations determining physical parameters of these spin chains are established. By solving these equations we can obtain the sets of values of these physical parameters. Examples of the chains with even and odd numbers of spins are presented. References

[1] Cirac J I, Zoller P, Kimble H J and Mabuchi H 1997 Phys. Rev. Lett. 78 3221

[2] Pellizzari T 1997 Phys. Rev. Lett. 79 5242

[3] Serafini A, Mancini S and Bose S 2006 Phys. Rev. Lett. 96 010503

[4] Nguyen Van Hieu, Nguyen Bich Ha and Duong Hai Trieu 2010 Adv. Nat. Sci.: Nanosci. Nanotechnol. 1 015001

[5] Lloyd S 2003 Phys. Rev. Lett. 90 167902

[6] Bose S 2003 Phys. Rev. Lett. 91 207901

[7] Christandl M, Datta N Ekert A and Landahl A J 2004 Phys. Rev. Lett. 92 187902

[8] Albanese C, Christandl M, Data N and Ekert A 2004 Phys. Rev. Lett. 93 230502

[9] Karbach P and Stolze J 2005 Phys. Rev. A 72 030301

[10] Nguyen Van Hieu 2009 J. Phys.: Condens. Matt. 21 273201

15. Neutron-scattering study of novel spin correlations in high-Tc superconductors

Masaki Fujita (1), Masanori Enoki (2), Satoshi Iikubo (3), Kazuyoshi Yamada (4)

(1) Institute for Materials Research, Tohoku University

(2) Department of Physics, Tohoku University,

(3) Graduate School of Life Science and Systems Engineering, Kyushu Institute of Technology

(4) World-Premier-International Research Center Initiative, Tohoku University

Antiferromagnetism in the doped cuprate Mott-insulator has been extensively investigated due to its rich physics and close relation with the high transition temperature (high-Tc) supercoductivity. A finding of a generic form of spin excitations showing the "hourglass" shape in the different superconductors $La_{2-x}(Sr,Ba)_xCuO_4$ (La-214) and $YBa_2Cu_3O_{6+\delta}$ (Y-123) strongly suggests a common role of spin fluctuations in the mechanism of high-Tc superconductivity. For the explanation of such novel spin excitations, two types of theoretical models were proposed. One is Fermi liquid model based on the itinerant fermions in which the spin excitations are explained through a response of quasiparticles. The other is so-called stripe model. In this model, the excitations correspond to the local spin dynamics in the antiferromagnetically-ordered spin domains which is segregated by self-organized hole carriers. Although above two scenarios provide different concepts for understanding the physical properties in high-T_c superconductors, the discrimination between them has not been successful experimentally. To make progress on above issue, it is useful to study appropriate reference systems. In this seminar, I present a result of high-energy neutron-scattering measurement on $Bi_2Sr_2CuO_{6+\delta}$ (Bi-2201) based superconductor. Bi-2201 system is a single-layer cuprate oxide, whose structure is similar to that in a prototypical high-Tc superconductor La-214. However, no information about the spin dynamics is so far reported for this system. This is due to difficulties in preparing high quality and sufficiently large samples. We have succeeded in growing single crystals and observed the spin excitation spectrum in a wide energy-momentum

space for the first time. The shape of excitation is quite similar to what observed in LSCO, namely, the hourglass-excitation exists in the superconducting phase of Bi-2201 system. Combine with the doping-dependence of low-energy spin excitation, I will discuss the "duality" of spectrum which is recently proposed for understanding the origin of hourglass-excitation.

16. Vortex current and induced magnetic fields originated from defects in metallic carbon nanotubes

Jisoon Ihm

Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea

In metallic carbon nanotubes, if defects exist, the electric current flow is expected to have characteristic spatial patterns depending on the nature of the defects. We perform first-principles calculations choosing the Stone-Wales defect as a prototypical example. The current-density loops are generated around the defects by the interference between conducting states and quasibound states at energies close to conductance dips originated from resonant backscattering. The direction of the loop current is reversed as the energy sweeps across the resonant energy. The current-density loops produce relatively strong magnetic fields in the near-field region including the inside of the tube and the fields decay in the far-field region as in the case of a magnetic dipole.

17. Anomalous collective excitations of cuprates

Chung-Pin Chou and T. K. Lee

Institute of Physics, Academia Sinica, Taipei, Taiwan

The properties of collective excitations in the strongly correlated systems have not been extensively studied so far. In this study we report variational Monte-Carlo calculations of collective excitation spectra for the extended t-J model in the superconducting phase. It is shown the presence of a particular low-energy collective excitation with modulations of charge, spin and pair field together. This anomalous collective excitation provides a better understanding of the

stripe-like states observed in our previous results for the t-J model and for the understanding of neutron experiments of cuprates.

18. Possible mechanisms of enhanced pairing gap near apical and dopant oxygens in cuprate

Mori M (1,2), Khaliullin G (3), Tohyama T (4), Maekawa S (1,2)

(1) Japan Atomic Energy Agency;

(2) JST-CREST;

(3) Max Planck Institute;

(4) Kyoto University

Scanning tunneling microscopy (STM) on Bi-based cuprate superconductors has revealed that a spatial variation of the pairing gap is correlated with a modulation of the apical oxygen position. We examine two mechanisms, by which apical oxygens can modulate the pairing interaction in the CuO_2 plane. One is a covalency between the in-plane band and apical oxygens, and the other is a screening of correlation by apical oxygen polarization. Their cooperative effect explains the experiment. Another STM experiment on the Bi-based cuprate has revealed an unexpected enhancement of the pairing correlations near the interstitial oxygen dopant ions. In this case, local screening effects modify the electronic parameters in the CuO_2 planes and strongly increase the magnetic exchange interaction. This enhances the spin pairing effects locally.

19. Effective action, magnetic excitations and quantum fluctuations in lightly doped single layer cuprates

Oleg P. Sushkov

University of New South Wales

We derive the effective action of the 2D extended t-J model and calculate quantum corrections using the action. There is a number of predictions of the theory including a Quantum Critical Point at doping about 10%. The results and predictions are compared with recent experimental data.

20. Electronic Anisotropy in Cuprates and Fe-Arsenides

Shin-ichi Uchida (1,2)

(1) Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033, Japan

(2) JST, Transformative Research-Project on Iron Pnictides, Tokyo 102-0075, Japan

Spectroscopic STM imaging of the pseudogap state in underdoped Bi2Sr2CaCu2O8+d has revealed a novel order parameter associated with the broken rotational symmetry -nematicity- within a CuO_2 unit cell [1]. The nematicity results from electronic inequivalence at the two oxygen sites, Ox and Oy, within each unit cell. This intra-unit-cell electronic nematicity may unify the understanding of the pseudogap state in high-Tc cuprates. The "nematic order" has a fairly long correlation length, 80-100 lattice constants. Superposed on it, a modulation with broken translational symmetry -smectic- is identified. The smectic correlation length is quite short, and is controlled by topological defects which are also responsible for the nanoscale inhomogeneity of the pseudogap distribution. A remarkable anisotropy in the in-plane optical conductivity is observed for detwinned $BaFe_2As_2$ single crystals. Consistent with the anisotropy in dc resistivity [2] conductivity in the a-axis direction (spins antiferromagnetically align) is higher than that in the b-direction (spins ferromagnetically align) up to 0.15eV, and is lower above it up to 2eV. The anisotropy sets on at the magneto-structural transition at Ts=143K, and overall spectral features are in agreement with the theoretical calculations for the stripe-AF ordered state [3]. However, some anomalous features including the anisotropic optical phonon response are not predicted by the theory and require involvement of orbital degree of freedom such as orbital ordering or orbital-polarized electronic states resulting from inequivalent Fe3dxz and 3dyz orbitals. These works have been done in collaboration with M. Nakajima, S. Ishida, T. Liang, T. Kakeshita, Y. Tomioka, T. Ito, C.H. Lee, H. Kito, A. Iyo, H. Eisaki, K. Fujita, Y. Kohsaka, J. Lee, E.A. Kim, and J.C. Davis.

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[3] Z.P. Yin, K. Haule, and G. Kotliar, arXiv:1007.2867 (unpublished).

21. Pairing fluctuations and quantum critical fluctuations in HTS cuprates

Jeffery Tallon

MacDiarmid Institute for Advanced Materials and Nanotechnology, and Industrial Research Ltd

Using thermodynamic data we analyse superconducting fluctuations near Tc to determine the "true" mean-field behaviour in a variety of HTS cuprates. A general picture emerges of nearly weak-coupling BCS-like behaviour across the entire superconducting phase diagram. We examine the thermodynamic implications of pairing being driven by quantum critical fluctuations and propose tests and limitations for their role in high temperature superconductivity

22. Common behaviors of unconventional superconductors indicating non-BCS condensation and spin-mediated resonant pairing

Yasutomo J. Uemura

Physics Department, Columbia University, New York, USA

In unconventional suprconductors, including high-Tc cuprates, FeAs, organic BEDT, A3C60 and heavy-fermion CeCoIn5 systems, we notice a few common behaviors which point towards novel condensation and pairing mechanisms. They include: (1) superconducting phase emerging adjacent to the competing antiferromagnetic / SDW states; (2) scaling of resonance-mode energy with Tc analogous to rotons in superfluid He; (3) scaling of the spin fluctuation energy scale with Tc; (4) scaling of the superfluid density with Tc in the underdoped region; (5) scaling of the superfluid density with Tc in the overdoped / pressurized region; (6) scaling of the specific heat jump C/T at Tc with Tc in the overdoped / pressurized

region. While (3) is expected for a BCS-like condensation, (2), (4), (5) and (6) point towards Bose-Einstein condensation where Tc is governed by the condensing boson density and mass. In particular, we notice that the spin fluctuation (mediating boson) energy scale is comparable to condensing charge energy scale (derived from superfluid density) in many of these systems, suggesting a resonant behavior in condensation and pairing. This may be a key concept to understand highly unusual non-BCS like behaviors (5) and (6) in the overdoped / pressurized regions of these unconventional superconductors. Scaling of Tc on the soft-mode energy (2), in addition to superfluid density (4) and (5), may be understood by BE condensation and BE-BCS crossover in the vicinity of magnetic competing states (1).

23. Possible π-junction in iron pnictide superconductors with antiphase s-wave pairing

Wei-Qiang Chen (1), Fengjie Ma (2,3), Zhong-Yi Lu (2), and Fu-Chun Zhang (1)

(1) Department of Physics, and Center of Theoretical and Computational Physics, the University of Hong Kong, Hong Kong, China;

(2) Department of Physics, Renmin University of China, Beijing 100872, China;

(3) Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China

We studied the Josephson junctions between two FeAs-based superconductors with antiphase s-wave pairing and a FeAs-based superconductor and a conventional s-wave superconductor, and found pi-junction under some circumstance. We proposed an experiment to probe the antiphase s-wave pairing and provided a possible explanation for the observed half integer flux quantum transitions in a niobium/polycrystal NdFeAsO loop.

24. Studying the properties of superconductors with ultracold atoms

Gilles Nogues

Institut Néel, CNRS and Laboratoire Kastler Brossel, Ecole Normale Supérieure

Atom chips are versatile experimental systems for trapping ultracold atoms and studying their behaviour very close to micro- or nanostructures. These devices are usually operated at room temperature with normal metal microwires. Recently microtraps made with superconducting materials have started to appear. In my talk I will present the Paris superconducting atom-chip experiment. Because of the specific properties of superconductors and low temperature, we have been able to observe very long trapping lifetime as the atoms are brought close to the surface, significantly longer than for normal metals. We have also shown that the trapping potential for the atomic cloud strongly depends on permanent current loops in the chip structures that can be induced at the time of transition to the superconducting state, hence displaying an hysteretic behaviour

25. 0.7 conductance anomaly: Multiple existence of Kondo impurities in a quantum point contact

Kang-Hun Ahn

Department of Physics, University of Bath, UK

The 0.7 conductance anomaly in a quantum point contact has attracted great attention because of its possible relevance to Kondo phenomena. I will introduce our recent investigation on the ground and excited states of interacting electrons in a quantum point contact using exact diagonalization method. We found that strongly localized states in the point contact appear when a new conductance channel opens due to momentum mismatch. These localized states form magnetic impurity states which are stable in a finite regime of chemical potential and excitation energy. Interestingly, these magnetic impurities have ferromagnetic coupling, which shed light on the experimentally observed puzzling coexistence of Kondo correlation and spin filtering in a quantum point contact.

26. Thermoelectric transport through a quantum dot: Interplay between FL and NFL behavior

M.N.Kiselev, V.E. Kravtsov and T.K.T. Nguyen

ICTP, Strada Costiera 11, I-34151 Trieste, Italy

We consider effects of magnetic field on the thermopower and thermo-conductance of a single-electron transistor based on a quantum dot strongly coupled to one of the leads by a single-mode quantum point contact. We show appearance of two new energy scales: the first one is proportional to the square of a sum up/down reflection amplitudes of the point contact; the second, minimal scale is proportional to the difference of up/down reflection amplitudes. While the first energy scale weakly depends on magnetic field, the second one, characterizing asymmetry of a spin-dependent scattering, is very sensitive to the field variation. Emergence of the minimal energy scale leads to a giant thermoelectric effect. We predict that the behavior of thermoelectric coefficients is consistent with the Fermi-liquid theory at temperatures smaller than minimal scale, while crossover from Non-Fermi-liquid regime associated with a two-channel Kondo effect to Fermi-liquid single-channel Kondo behavior can be seen at intermediate temperatures.

27. Density of states of graphene in the presence of strong point defects

Chung-Yu Mou

Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

The density of states near zero energy in a graphene due to strong point defects with random positions are computed. Instead of focusing on density of states directly, we analyze eigenfunctions of inverse T-matrix in the unitary limit. Based on numerical simulations, we find that the squared magnitudes of eigenfunctions for the inverse T-matrix show random-walk behavior on defect positions. As a result, squared magnitudes of eigenfunctions have equal a priori probabilities, which further implies that the density of states is characterized by the well-known Thomas-Porter type distribution. The numerical findings of Thomas-Porter type distribution is further derived in the saddle-point

limit of the corresponding replica field theory of inverse T-matrix. Furthermore, the influences of the Thomas-Porter distribution on magnetic and transport properties of a graphene, due to its divergence near zero energy, are also examined.

28. Non-BCS superconductivity for underdoped cuprates by spin-vortex attraction

Lu Yu

Institute of Physics, Chinese Academy of Sciences

Within a gauge approach to the t-J model, we propose a new, non-BCS mechanism of superconductivity for underdoped cuprates. The gluing force of the superconducting mechanism is an attraction between spin vortices on two different Néel sublattices, centered around the empty sites (holes), which can be described in terms of fermionic holons. The spin fluctuations are described by bosonic spinons with a gap originating also from the spin vortices. Due to the no-double occupation constraint, there is a gauge interaction between holon and spinon, through which the spin vortex attraction induces the formation of spin-singlet (RVB) spin pairs with a lowering of the spinon gap. Lowering the temperature there appear two crossover temperatures. At the higher crossover, a finite density of incoherent holon pairs are formed, and it is identified with the pseudogap temperature. At the lower crossover temperature, a finite density of incoherent spinon RVB pairs are formed, and it is identified with the appearance of the Nernst signal. The true superconducting transition occurs at an even lower temperature, via a 3D XY-type transition. The superconducting mechanism is not of BCS-type, and it involves a gain in kinetic energy (for spinons) coming from the spin interactions. The main features of this non-BCS description of superconductivity agree with the experimental results in underdoped cuprates, especially the contour plot of the Nernst signal.

29. Real-Time Dynamics of Correlated Electronic Systems

Naoto Nagaosa

Dept. Applied Physics, The University of Tokyo

The real-time quantum dynamics of the correlated electronic systems is an important but notoriously difficult problem for theories, and has denied the full understanding. Recently, there are several experimental advances. Especially, even though the optical activity of the magnetic systems has been the subject since long ago, the optical manipulation of magnetism is the topic of intense interest only recently. Also the photo-induced phase transitions are now studied in a variety of systems. In this talk, I will discuss some of our recent works related to the real-time dynamics of the correlated systems. (i) Photo-induced chirality switch in multiferroics RMnO3 In RMnO3, the ferroelectricity associated with the non-collinear magnetic structure is realized, and its dynamical properties including the electromagnon have been studied. We have developed the quantitative theory of electromagnon optical spectra (OS) by constructing the detailed microscopic spin Hamiltonian consistent with the phase diagram. It turned out that the nonlinear interactions play important role to reproduce the observed OS. Based on this spin Hamiltonian, we study numerically the effect of intense pico-second optical pulses on the magnetic system. It is found that the optical switching of the vector spin chirality is possible by tuning the pulse-width and intensity though the nonlinear electromagnon excitations. (ii) Photo-induced metal-insulator transition in spin-electron coupled system We present a model where the electrons are coupled to classical spins, i.e., double exchange model, to simulate the quantum real-time evolution of the electronic system combined with the classical spin dynamics. This model has the ferromagnetic metallic and antiferromagnetic insulating states as two nearly degenerate ground states. By this model, we analyze the real-time dynamics of the photo-induced metal-insulator transition including the nucleation process, non-adiabatic transitions, space-time pattern formation, and appearance of the spiral magnetic structure. These works have been done in collaboration with M. Mochizuki, N. Furukawa, and W. Koshibae.

30. Quantum-ensured comparative voting and anonymous broadcast channels

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We want to explore methods for quantum communication that protect privacy. These arose initially out of a study of quantum voting. In quantum voting, one has an authority, who prepares ballots and who counts the votes, and voters, who cast votes. We suggest schemes that allow the authority to determine how many ``yes'' and ``no'' votes there are, but not how any individual voter voted. Cases of two, four, and an arbitrary number of voters are considered. Possible realization with linear optics is discussed and the vulnerability of these schemes to eavesdropping is examined. Comparative voting schemes are closely related to cryptographic constructs called anonymous broadcast channels. This is a multi-party channel in which anyone can send a message to everyone else, but the source of the message will not be known. In order to create a quantum anonymous broadcast channel, we need a multi-particle quantum state in which users can, by local operations, create the same global quantum state. The simplest example is given by an n-qubit Greenberger-Horne-Zeilinger state where the information to be conveyed anonymously to participants in the network is encoded in the phase differences between the component states. A quantum anonymous broadcast channel with the information encoded in the weights of the component states can be set up as well, via rotations of an n-qubit symmetric state. Finally we consider a scheme based on a two-mode squeezed vacuum.

31. Novel Spin-Orbit Physics in 5d Transition Metal Oxides

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Recently we have reported the unique influence of spin-orbit coupling on 5d transition metal oxides. A novel jeff=1/2 state is manifested in the Mott insulating state of Sr_2IrO_4. The electron correlation combined with strong spin-orbit (SO) interactions under a large crystal field present is responsible for the observed peculiar electronic and magnetic properties. Based on LDA+SO+U calculations including both on-site Coulomb and spin-orbit interactions, we have investigated a series of 5d Ir oxide compounds including Sr_2IrO_4, Na_2IrO_3, and $LixIr_2O_4$. The results show that there is an interesting competition between local lattice distortion and spin-orbit coupling, which controls the degree of jeff=1/2 component in the state near EF. We will discuss the nature of its electronic structure and properties and a possible topological insulator based on Ir.

32. Dephasing, disorder and interaction effects in 2D topological insulator

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The influence of dephasing on the quantum spin Hall effect (QSHE) appeared in 2D topological insulator (TI) is studied. In the absence of dephasing, the longitudinal resistance in a QSHE system exhibits the quantum plateaus. We find that these quantum plateaus are robust against the normal dephasing but fragile with the spin dephasing. Thus, these quantum plateaus only survive in mesoscopic samples. In addition, we define a new spin Hall resistance that also exhibits quantum plateaus. In particular, these plateaus are robust against any type of dephasings and therefore, survive in macroscopic samples and better reflect the topological nature of QSHE. We also study the disorder effect on the transport properties in QSHE. We confirm that

at a moderate disorder strength, the initially un-quantized two terminal conductance becomes quantized, and the system makes a transition to the novel topological Anderson insulator (TAI). Conductances calculated for the stripe and cylinder samples reveal the topological feature of TAI and support the idea that the helical edge states may cause the anomalous quantized plateaus. The influence of disorder is studied by calculating the distributions of local currents. Base on the above-mentioned picture, the phenomena induced by disorder in the quantum spin Hall region and TAI region are directly explained. In addition, we study the effect of the electron-electron interaction in 2D topological insulator, particularly on the transition between TI and Mott insulator.

33. Rigidity in amorphous networks: from simple sulphides to complex phase-change tellurides

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In amorphous networks where the 8-N (octet) rule holds (N being the number of s and p electrons), particularly sulphur and selenium based systems, rigidity theory offers a practical computational scheme using topology, namely the Maxwell counting procedure, and has been central to many contemporary investigations on non-crystalline solids. It has led to the recognition of a rigidity transition which separates flexible glasses, having internal degrees of freedom that allow for local deformations, from stressed rigid glasses which are "locked" by their high bond connectivity. What happens if sulphur or selenium is replaced by an heavier element such as tellurium which leads to an increase electronic delocalization and more complicated (and non-obvious, e.g. distorted octahedral and possibly tetrahedral) local structures? Here I will show how ab initio Molecular Dynamics is able to provide a precise estimate of bond-bending and bond-stretching constraints from the accumulated trajectories. We first stress the need to improve electronic models of chalcogenides as highlighted by the benchmark case GeSe2 and then apply these new methods to "heavier" chalcogenides including phase-change SnSe2 and Ge-Sb-Te alloys which represent the archetypal systems of the DVD technology.

34. Anderson-Haldane Liquid: a novel Resonating Valence Bond Metallic State

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Resonating valence bond states, in addition to being seats of high Tc superconductivity, are seats of unusual metallic states. Under doped pseudo gap phase and optimally doped metallic phase of high Tc cuprates exemplify this. We show that, generically, lightly doped RVB states become, what we define as an Anderson-Haldane (AH) liquid, where the doped holes have an unconventional (Haldane) exclusion statistics of 3/2. This is, in certain RVB background the doped physical hole (charge +e and spin-half) is a weakly bound (spin-charge locked, in the sense of Anderson) composite of a holon and a spinon. It has an exclusion statistics of 3/2 = 1 + 1/2, a sum of exclusion statistics of holon and a spinon. Consequently each doped hole, a fermion, occupies 3/2 of k-space volume than that occupied by an usual fermionic hole in a band insulator. AH liquid behaves like a fermi liquid for all practical purposes. However it violates Luttinger theorem and volume of fermi surface is determined by Haldane exclusion statistics parameter and hole density. Further, its shape is determined mostly by super exchange interactions. We also discuss, starting from an AH liquid, how one reaches i) the superconducting state and ii) the over doped regime with a large fermi surface. Many of the quantum oscillation features seen in under doped cuprates can be explained by our theory. Relevance of our Anderson-Haldane liquid state for other systems such as the organic and Fe arsenide family of superconductors will be pointed out.

35. Influence of Phonon Confinement on Absorption Influence of Phonon Confinement on Absorption Power and Line-Widths in Rectangular Quantum Wires

Le Dinh, Le Quoc Anh and Tran Cong Phong

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Based on state-independent projection operator technique (SIPOT) we obtain analytical expressions of absorption power in rectangular

quantum wires (RQW) due to electron-longitudinal optical phonon (LO-phonon) interaction. Both electrons and phonons are confined in the wire. The numerical results are presented for GaAs/AlAs RQW. From graphs showing the dependence of the absorption power on the frequency of external laser field we obtain line-widths as profile of the curves. The dependence of the line-widths on the temperature, the wire's size is obtained. Comparison between the value of the absorption powers and the line-widths in the case of confined phonons and bulk phonons is discussed.

36. First-principles investigations of the dielectric properties of Silicon Nitride films

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We have investigated the dielectric properties of silicon nitride thin films with thickness below 6 nm, by using density functional theory calculations. We find a substantial decrease in the static dielectric constant of crystalline films, as their size is reduced. The variation in the response in proximity of the surface plays a key role in the observed decrease. In addition, amorphization of the films may bring further reduction of both the static and optical dielectric constants.

37. Light Absorption by excitons in bilayer parabolic quantum dots

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We study theoretically excitons in bilayer two-dimensional parabolic quantum dots by using an unrestricted Hartree-Fock method. In the model electrons and hole are in planes spatially separated by distance d. The charging effect on electronic structure of the system is studied numerically in function of distance between two layers. The light

absorption by charged excitons is calculated and shown in the dependence of distance between two layers.

38. Dirac electrons under a tunable potential barrier in graphene.

Tran Nguyen Dung, Nguyen Hai Chau

Institute of Physics, VAST

We study the electric transport properties of Dirac fermions under a tunable potential barrier in graphene, taking into account the nonlinear screening effect in the junction regions. Depending on the top gate and the back gate voltages the considered system may behave as a npn, nn'n, pnp, or pp'p heterojunctions. For all these heterojunctions the conductance/resistance and the shot noise are calculated and analyzed in details in the ballistic regime, using the T-matrix approach. In the diffusion regime when the conductance of the double-junction is practically determined by that of a single one the obtained junction resistance describes quite well the experimental data reported by Huard et al. [Phys. Rev. Lett. 98, 236803 (2007)].

39. Mechanism of Solidification of Vitreous GeO_2 Nanoparticles

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Solidification of vitreous GeO_2 nanoparticles is studied in details via detecting the solid-like atoms using MD simulation upon cooling from the melt. Solid-like atoms are identified by applying the Lindemann-like freezing criterion and we found they occur in the model at the higher temperature than the glass transition point. They have the tendency of forming clusters and span throughout the model leading to the formation of solid-like regions. Moreover, we can answer the question that whether the first solid-like cluster grows at the surface or in the core of GeO_2 nanoparticles. Nevertheless, the size-dependence of structure upon cooling from the melt is studied in details.

40. Structural properties of simulated liquid GaxAsy

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The structural properties of liquid and amorphous gallium arsenide have been studied using the molecular dynamics (MD) method. Simulations were done in the basic cube under periodic boundary conditions containing 3000 ions for GaAs, $GaAs_2$, Ga_2As models. The micro-structure of systems has been analyzed through partial radial distribution functions (PRDFs), coordination number distributions, bond-angle distributions and inter-atomic distances. The evolution of structure upon cooling from the melt of Ga-As was observed and discussed. We found that calculated data agree well with the experimental ones and with those obtained previously in other simulation works. Moreover, temperature dependence of these distributions was obtained.

41. Calculations of pressure dependence of EXAFS cumulants in zinc-blende semiconductors

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The statistical moment method (SMM) has been developed to study the pressure dependence of the extended x-ray absorption fine structure (EXAFS) cumulants in zinc-blende semiconductors. Analytical expressions of the first two EXAFS cumulants and anharmonic factor have been derived. The equation of state for these semiconductors has been obtained using which the pressure dependence of lattice constants, the change of volumes and bulk moduli have been estimated. Numerical results for a series of zinc-blende type semiconductor have been performed and compared to

available theoretical and experimental data showing the good agreement.

42. Optical sum frequency microscopy of cellulose fibers

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We used a sum frequency (SF) confocal microscope to investigate cellulose fibers. The sample was cellulose I fibers contained in filter paper. Sum frequency spectrum showed a prominent peak of asymmetric CH2 stretching mode at ~ 2945cm^-1. The CH stretching vibration in the pyranose ring at 2890cm^-1 was very weak probably because SFG from CH groups cancel each other due to their highly symmetric configuration in the polymer structure. The result is in contrast with the Raman spectrum of cellulose I fibers showing a dominant CH stretching peak [1]. The SF intensity image of the cellulose fibers was observed by a confocal sum frequency microscope. Different bunches of cellulose microfibrils were found to have different second-order nonlinear optical susceptibility. The polarization dependent SF images indicated that methylene groups have a preferential orientation in the fiber.

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43. Photocatalytic activity of transition-doped TiO2-d nanobelts synthesized by metalorganic chemical vapor deposition

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An efficient photocatalytic activity of the TiO_2 has attracted extensive interest for various applications such as the electrodes of solar cells, the elimination of pollutants, and the splitting of water for hydrogen fuel. Recently, much attention has been focused on the use of 1-D TiO_2 nanostructures such as nanotubes and nanobelts to enhance the reactivity and avoid several problems of TiO_2 powders and thin films. However, the wide bandgap energy (~3.0-3.2 eV) of TiO_2 limits its photocatalytic reaction to ultraviolet light. To enhance the efficiency in the visible light range, studies on dye sensitization or doping have been intensively performed. An alternative approach can be utilizing oxygen vacancies at various shallow level energies in TiO_2 bandgap, which can lead visible-light luminescence and photocatalysis. In this study, we report some results of transition metal (Co, Fe, Sr)-doped TiO_2- nanobelt growth using metalorganic chemical vapor deposition (MOCVD) and their visible-light photocatalytic characteristics. TiO2 nanobelts were self-catalytically grown without the use of any metal catalysts on bare Si (100) substrates at 510 oC by MOCVD. The (C11H19O2)2(C3H7O)2Ti was used as a titanium metalorganic (MO) source and bubbled at 200 0C with the gas flow rate at 150 cm3/min. The chamber pressure was fixed at 1.2 Torr. To realize visible-light photocatalytic activity, transition metals (Sr, Fe, and Co) were in-situ doped in the TiO_2-d nanobelts, respectively by using Sr, Fe, and Co MO sources. The photocatalytic activities of TiO_2-d nanobelts were evaluated by the decomposition of methylene blue under both UV and visible light irradiation. The TiO_2-d nanobelts exbihited high visible-light photocatalytic activity. We will further discuss the growth mechanism and photocatalytic characteristics of the undoped and transition metal-doped TiO_2-d nanobelts.

44. Preparation of Water-soluble Multi-walled Carbon Nanotubes Using Simple Oxidizing Agent

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A simple acid-treated method for preparing water-soluble multiwalled carbon nanotubes (MWCNTs) is reported. Ammonium persulfate solution -(NH4)2S2O8 (APS) was used as oxidant to modify surface

of MWCNTs at 80 oC with different treated times (1-24 hr). TGA and FT-IR were used to characterize the amount and types of oxygenated functional groups on modified MWCNTs. FT-IR spectra show carboxylic and lactone groups are the main oxygenated functional groups of acid-modified MWCNTs. TGA measurements also supported the results of FT-IR. APS-modified MWCNTs are well dispersed in aqueous system for several months. The modifying process reported here is simple, low-cost and eco-friendly method to integrate MWCNTs into further biological applications.

45. The Nonlinear Electrical Conduction in Parabolic Quantum Wells

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The dc electrical transport in a quantum well with parabolic confinement potential $U(z)=m\omega_{z}z^{2}/2$ (where m and ω_{z} are the effective mass of electron and the confinement frequency in z direction, respectively) in the presence of a very strong magnetic field $\vec{B}$ perpendicular to the electric field that is taken in the x direction is considered analytically. The scattering by optical phonons is investigated at high temperatures and strong magnetic fields (nonlinear transport), while the scattering by acoustic phonons is considered at low temperatures and weak electric fields (linear transport). The dependence of the conductivities (or currents) on the magnetic field, the confinement frequency, and the temperature is shown explicitly.

46. Spin dependent transport in ferromagnetic gate graphene structures

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Because of its high carrier mobility [1], graphene appears to be a very promising material for designing high performance devices. Besides, due to very weak spin orbit interaction, which leads to a long spin flip length (~ 1\mu m), it also offers a good potential for spintronic applications [2]. Using the non-equilibrium Green's function method, we have studied the spin dependent transport in different graphene-based structures including a ferromagnetic gate. The most interesting property of charge carriers in graphene is the chirality, which leads to some unusual phenomena, especially regarding tunnelling and confinement [3-5]. In gated structures, these properties lead to conductance oscillations as a function of the barrier height. As a consequence, when inducing a spin splitting in the gated region, we find that the spin polarization has an oscillatory behaviour with respect to the barrier height, which suggests a high controllability of spin transport using the gate voltage in ferromagnetic graphene structures [4,6,7]. Moreover, due to strong resonant effects, the nearly perfect polarization of spin dependent current can be observed in armchair graphene nanoribbon structures when the energy bandgap is large enough or using normal conducting leads [6]. A similar behaviour is observed in bilayer graphene structures [7]. The sensitivity of obtained results to the device parameters has been also investigated. Our study provides some suggestions likely to be helpful for designing efficient spintronic devices. References:

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47. Study on the formation of nano-structure for TiO2 material

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The influence of the technology conditions on the formation of the nano-structure TiO2 system which was prepared from the materials such as oxygen TiO2, TiO2+2% wt was investigated. At the optimal conditions, the materials are single phases with the rutile structure and the size of nano-particle is about from 50 nm to 70 nm. We predicted the theoretical PL and magnetic properties by Density Functional Theory and compared them with data obtained from measurements.

48. Photoluminescence of ZnO nanocolloid

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The paper presents our results on characteristic photoluminescence of ZnO nanocolloid. The ZnO nanoparticles were fabricated by wet chemical route, then separated by high-power ultra-sound in solution with organic solvent. The colloid was obtained from two main solutions, one containing the nanoparticles and another containing the surfactant (surface-active-component). The thin films were fabricated at room temperature on the silicon substrate and were subjected for absorption, photoluminescent measurement. The experimental results were compaired with the theoretical results obtained from Density Functional Theory using the effective medium simulation for solvent

of different dielectric constant. It showed the observable red-shifts, variations of band-gaps and a very large change in luminecent intensity of the main luminescent line.

49. Synthesize and research Au coated APTES/SiO2/Fe3O4 nanoparticles by seed-mediated method, potentially application in biomedicine.

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We synthesized and researched Au coated APTES/SiO2/Fe3O4 nanoparticles by seed-mediated method. The first, SiO2 coated Fe3O4 nanoparticles were prepared by sol-gel. Then, these nanoparticles were functioned by APTES to produce NH2- which leaves out. Due to this function, it helped conjugating with gold nanoparticles with sizes less than 10 nm, which produced initial seed gold. Finally, gold salt Au3+ was reduced by THPC on seed gold - APTES/SiO2/Fe3O4 to produce homogenous gold layer. These resulted nanoparticles had high stability and novel optical and magnetic properties, potentially application in biomedicine.

50. Novel simulations on chain-like formation of ferrofluids: influence of anisotropy.

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In this report, we use the Monte Carlo method to study the chain-like formation of mono-dispersity ferrofluid. The main cause of chain-like formation is the dipolar interaction between particles, however, in the presence of the intrinsic anisotropy, this phenomenon is modified (ACS Nano Vol. 3, No. 6, pp. 1539-1547, 2009). We will investigate the influence of the anisotropy strength as well as the alignment of

easy axes on the chain-like formation. The snapshot and the pair correlation function are used to analyze the configuration of ferrofluid.

51. Nanoscale crystalline nucleation of supercooled liquid gold

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Base on Molecular Dynamics method under periodic boundary conditions to mimic the characteristics of bulk material form, we create a model with 3000 atoms in order to investigate the crystallization of supercool liquid gold. The liquid gold was cooled down from 2500K to 50K at three different cooling rates by using Erkcoc's pair-interaction potential. Structure of models was studied via radial distribution function, interatomic distance, coordination number and Honeycutt-Andersen analysis. In addition, we found temperature dependence of mean-square displacement of atoms, Lindemann ratio and potential energy. We found that at low cooling rate the crystallization occurs in the system. We found the onset of crystalline nucleation in supercooled liquid Au via clustering of solid-like atoms at nanoscale.

52. Investigation of the Glass-to-Liquid Process of Monatomic Lennard-Jones glass

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Melting of Lennard-Jones (LJ) glass has not been well understood for the reason of whether there is glass-liquid transition or glass-crystal-liquid transition. For that reason, we heated up monatomic Lennard-Jones glass at three different heating rates using molecular dynamics simulation to study in details about the glass-to-liquid process. Structure of LJ systems has been analyzed in details via radial distribution function (RDF), mean atomic distances, coordination number and bond-angle distributions. We used Lindemann melting-

like criterion to detect liquid-like atoms in order to investigation the glass-to-liquid process. Temperature dependence and clustering of liquid-like atoms have been analyzed in addition to corresponding changes in various thermodynamic quantities. Depending on the heating rate used in simulation, one can observe glass-liquid or glass-crystal-liquid transitions. Keywords: glass-to-liquid transition, monatomic Lennard-Jones glass, MD simulations

53. High TC phase transition in Li-doped Bi-2223 thin films grown by pulse laser deposition method

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We have investigated the effect of Li doping on the superconducting properties of Bi-2223 thin films deposited on single-crystalline (100) STO substrate using pulsed laser deposition (PLD), post annealed at 850 Â°C for various lengths of time. X-ray diffraction measurements showed that all the films are c-axis oriented. Resistivity measurements showed that the superconducting onset transition temperature (Tcâ^'onset) and zero resistive temperature (Tcâ^'zero) for the best films are 115 K and 95 K, respectively. The highest critical current density obtained from magnetic measurements for the undoped film is Jc = 4,2 Ã— 106 A cmâ^'2 in 0.5 T magnetic field at 20 K. Among the Li-doped films, the 7 wt% Li-doped Bi-2223 film showed highest Tc=115 K, which is higher than that for the undoped Bi-2223 film.

54. Computer Simulation of the Diffusion Processes in one-Dimensional Disordered Systems

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Monte Carlo simulations, the one-dimensional diffusion motion of a chain of N particles is studied to determine its diffusion coefficient.

The diffusion coefficient D can be determined by slope of the versus tn curve, but the accuracy of this method depends on the length of the chain and in particular will be very difficult to apply for two- and three-dimensional models because of the increment of computing time. In this study, non-external and external force methods are applied to study the mechanism of diffusion in a linear chain of sites. The external force method is applied to short-chain and using periodic boundary conditions. The non-external force method is applied to long chain and without boundary conditions. Investigation shows that, results calculated by these two methods are in good agreement with each other. It means we can reduce computing time by using external force method instead of non-external one. This is the basis for the study of diffusion mechanisms on the two-dimensional, three-dimensional models. Studying also refers to dependence on the Arhenius law of the diffusion process and effect of distribution of energy level to the diffusion coefficient. .

55. Optically detected electrophonon resonance effects in compositional semiconductor superlattices

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The electrophonon resonance (EPR) and optical detected electrophonon resonance (ODEPR) effect in compositional semiconductor superlattices (CSSL) are investigated by using the quantum kinetic equation (QKE) for electrons in the case of electron - optical phonon scattering. General analytic expressions for absorption coefficient are obtained. We also obtain the selection rules for transition and the photon energy dependence of ODEPR condition for a specific CSSL. In particular, anomalous behaviors of the ODEPR effect such as the shifting of ODEPR peaks for incident photon energy are discussed. Comparing this result with the doped semiconductor superlattices result we see that the ODEPR effect raises a possibility of detecting experimentally electric subbands in CSSLs.

56. Calculation of Temperature Dependence of Absorption Line-Widths in Cylindrical Quantum Wires

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In this paper, we apply the theory of optical conductivity for an electron-phonon system, that has appeared recently [Phys. Rev. B 65, 195113 (2002)], to calculate the temperature dependence of absorption line-widths in cylindrical quantum wire (CQW). In the first time, the graphic dependence of absorption power (AP) on the photon energy and the shape CQW is achieved computationally for a specific CQW. From graphs of the AP we obtain linewidths as profile of curves. The results show that the line-widths increase with the temperature increasing.

57. A Theory of Linewidth for Nonlinear Optical Conductivity in Rectangular Quantum Wires

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General expressions for nonlinear absorption power (NLAP) are obtained by using projection operator technique in rectangular quantum wires (RQW) for the case of electron-optical phonon scattering. Two-phonon process is included into the result. In the first time, the graphic dependence of NLAP on the photon energy and the wire's size is achieved computationally for a specific RQW. From the graphs of the NLAP we obtain half-linewidths as profile of curves. The results show that the half-linewidths increase with temperature and decrease with the size of RQW. Comparing this result with the two-dimensional result we see that the widths in the one-dimensional electron system are larger than those in the two-dimensional case. This implies that the scattering becomes stronger in one dimensions

58. Optically Detected Electron Energy Spectrum in Cylindrical Quantum Wires

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Optically detected electron energy spectrum (ODEES) in cylindrical quantum wires (CQW) is investigated by using the quantum kinetic equation for electrons. Due to the appearance of peaks in absorption spectrum satisfying the condition of electron-phonon resonance we obtain a relation between photon energy, distance of the two peaks, and electron subbands in the CQW. The importance of the result is that the splitting of peaks for incident photon energy can be used to detect electron energy spectrum in a CQW. The obtained ODEES do not depend on the temperature.

59. Rate of phonon excitation and conditions for phonon generation in rectangular quantum wires

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We present a theory of phonon generation via the Cerenkov effect in rectangular quantum wires (RQWs) based on the quantum kinetic equation for phonon population operator. Analytical expressions for the rate of change of the phonon population and conditions for phonon generation are obtained. Both electrons and phonons are confined. Numerical results for a specific RQW show that the amplitude of the laser field must satisfy additional conditions that are different in comparison with those of the generation of bulk phonons.

60. White Light Emission from Nano-structured Materials

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In response to ever-increasing energy demands and subsequent costs, a tremendous emphasis is being placed on energy saving, solid state lighting devices in the form of light emitting diodes, or LED's. White LED lightning is rapidly evolving technology, now virtually certain to someday replace traditional lighting because it possesses several advantages compared to incandescent bulbs or fluorescent tubes. With incandescent bulbs, electric current resistance causes tungsten filaments to heat up and glow, with 90 percents of the energy wasted as heat. In fluorescent lamps, electricity is used to excite mercury vapour, producing shortwave UV light that is converted to visible light when it strikes the tube's phosphor coating, with about 80 percents of energy wasted as heat. In this work, we demonstrate a high-level overview of solid-state lighting, with an emphasis on white lighting suitable for general illumination. We characterize in detail solid-state lighting's past, present and potential-future evolution using various performance and cost metrics, with special attention paid to inter-relationships between these metrics imposed by human factors, technology and economic considerations.

61. Investigation of Optical Response in Antiferromagnetic Phase of Iron Pnictides with Mean-Field Approximation

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Since the discovery of high-temperature iron pnictide superconductors, many studies about iron pnictides have been carried out. The parent compound has antiferromagnetic phase, and it implies the close connection between superconductivity and antiferromagnetism in iron pnictides. In order to elucidate the mechanism of high-temperature superconductivity, the understanding of electronic states in the antiferromagnetic phase is desired. Especially, the study of orbital properties in the magnetically ordered state is crucial for the understanding of this multiband system. To investigate the band structure, one makes use of optical responses such as optical conductivity and Raman scattering. Recent experimental researches

have pointed out in-plane anisotropy of electric transport properties [1,2,3]. In this paper, we focus on the anisotropy of optical conductivity arising from interband transition. We investigate the optical conductivity in BaFe2As2 by means of mean-field calculations. We find that the excitation spectra of interband transition show anisotropic feature in the antiferromagnetic phase reflecting its anisotropic electronic structure. The calculated results of the optical conductivity are analyzed in terms of the band structure and the anisotropy of Fermi surface. The analyses assert that the symmetry of the orbitals of initial state and final state in transition is important for the anisotropy of optical conductivity. In addition, we discuss Raman scattering in the (aa), (ab), (xx), (yy) and (xy) spectra, where the a and b axes are parallel to the Fe-As-Fe and the x and y axes are the bisecting directions. 1 J.-H. Chu et al., Science 329, 824 (2010) 2 M. A. Tanatar et al., Phys. Rev. B 81, 184508 (2010) 3 A. Dusza et al., arXiv:1007.2543

62. Properties of Polypyrrole and Single Wall Carbon Nanotubes Composites

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Single wall carbon nanotubes (SWNTs) were used as a component in SWNTs/PPy nanocomposites synthesized by in-situ chemical polymerization. The present of SWNTs modifies the morphology of PPy which is more symmetrically growth in the spherical form with radius 1-2 Î¼m. Raman and FTIR spectra show the PPy undergoes a transition from polaron to bipolaron state, i.e., indicate an increase in conductivity of PPy. The adsorption band around 340 nm (TT*- TT transition) in UV-Vis spectra exhibits a red shift indicating a relocation in PPy band gap. Upon exposure to oxygen the conductivity of SWNTs/PPy exhibits a change more than 10 and 50 times in comparison to that of neat PPy or SWNTs, respectively

63. Structure and Properties of Ca0.85Pr0.15Mn1-yRuyO3 (y = 0-0.2) Thin Films Fabricated by PLD Technique

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The Ca0.85Pr0.15Mn1-yRuyO3 (y = 0, 0.04, 0.08, 0.12, 0.16, and 0.20) perovskite thin films were prepared by Pulsed Laser Deposition (PLD) technique. The X'ray diffraction (XRD) analysis revealed that the samples were single phased with orthorhombic structure. The scanning electron microscopy (SEM) images indicated that the samples were composed of homogeneous grains. The Hall-effect measurements showed that the carrier density and Hall mobility of films increased with increasing Ru-doped content. The magnetic field dependence of magnetization at various temperatures were measured by using the superconducting quantum interference device (SQUID) and showed that the increase of Ru-doping content induced the large Delta S change in broad range of temperature. This demonstrates a possible application of these materials in cooling devices as the relative cooling power (RCP) is proportial to -(dS)max- dTFWHM (where dTFWHM is the full-width at the half maximum of dS). Keywords: Perovskite, Hall Effect, thin film, PLD.

64. Efficient 3D Poisson solvers using post-BICGSTAB algorithms

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This paper presents new-built efficient 3D Poisson solvers using post-BICGSTAB algorithms of BICGSTAB (L) and enhanced BICGSTAB (L). The efficiency of these solvers and comparable solvers are tested on Windows computers. It is showed that these solvers have a lot of advantages of convergent characteristics, memory accumulation and speed compared to solvers based on LU decomposition, Gauss's elimination, Jacobi and Gauss-Seidel iteration algorithms.

65. Electronic structure of a molecular magnet from salicylate based copper complex

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The electronic structure of the metallo-organic compound Cu(SA)2(2-PM)2 (2-PM is 2-pyridylmethanol) is presented. The calculation was performed using the Density Functional Theory with unrestricted spin polarized model and large wave function basis sets which include the polarized and diffuse functions. The single point energy calculation for the isolated molecule gave the HOMO-LUMO separation of 3.8 eV and the LDA+U band structure calculation showed the band gap of only 0.38 eV. The calculated magnetic moment per molecule is comparable to the experimentally observed value. Keywords: Molecular magnet, DFT, Electronic structure

66. Orange photoluminescence of nanosize materials based ZnS

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ZnS and Mn2+ doped ZnS nanocrystals were synthesized by wet chemical method. All obtained samples are single phase with sphalerite crystal structure. The average particle size is about 3-5nm. The optical absorption spectra of ZnS sample are blue shifted compared to that from the bulk material, reflecting a nano size effect. The absorption edge of the ZnS:Mn2+ samples shift to long wavelength with increasing Mn2+ content. The photoluminescence intensity at 588 nm of ZnS:Mn2+ samples reached a maximum in the sample with 0.9% Mn2+. The orange emission of samples is improved by the polymer coating process. The thin films ZnS and ZnS:Mn2+ were deposited on glass substrates by a spin-coating technique. The films have a single sphalerite phase with good crystallinity. The average crystallite size is about 3- 5 nm.The treatment temperature clearly influenced on film structures and it should be not more than 200oC. The influences of a preparation condition on the photoluminescence properties were discussed.

67. Electronic Structure of EU- DOPED CaO by Density Functional Theory

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We report the ab initio calculation of electronic structure of Eu-doped CaO. The obtained results appeared in a very good agreement with experimental data and predicted the existence of a ferromagnetic state for one doped compound. The light doping could induce the electron trapping property and the heavy doping the half-metallic ferromagnetic state.

68. Transparent thin film nanostructure device

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Indium tin oxide (ITO) is one of the most widely used transparent conducting oxides (TCO) because of its electrical conductivity and optical transparency.We have grown "all oxide" transparent p-n junction thin film nanostructure device by using chemical solution deposition and e-beam evaporation onto SiO2 substrate. The oxide p-n junction was characterized by GIXRD, AFM, UV-Vis. spectroscopy and I-V measurements. Combined GIXRD and AFM confirm phase pure, mono-disperse 30 nm NiO and ITO nanocrystallites. More than 70% optical transparency is achieved across 160 nm thick p-n junction. The forward bias current is greater than the reverse bias current by approximately a factor of 104 in the measured voltage s weeping range. A small leakage current as low as 12 nA was observed at a reverse bias of -5 V. Previously, Tonooka and co-authors reported the average turn on voltage of their n-ZnO / p-Cu-Al-O diode ~ 0.5 V,

which is higher than our p-NiO/n-ITO diode. This is mainly because of the large variations in the carrier concentrations as well as larger lattice mismatch between the oxides forming the p-n junction.The observed optical and electrical properties of oxide transparent diode are attributed to the heteroepitaxial nature and carrier diffusion at the junction interface.

69. Coherent potential approximation study of transport properties in the ionic Hubbard model on half-filled bipartite lattice

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The electronic phase transitions and conductivity of the ionic Hubbard model on half-filled bipartite lattice are studied within the coherent potential approximation (CPA). It is shown that at low temperature the two insulator phases are separated by a metallic phase for week to intermediate values of the ionic energy Δ . For large Δ the metallic region shrinks to a line in the $U - \Delta$ phase diagram. The conductivity as a function of temperature and model parameters is also numerically calculated and discussed.

70. Spin orbit coupling in graphene nano-ribbons

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The spin orbit coupling (SOC) is considered very weak in graphene sheets. For graphene nano-ribbons (GNRs) the edge construction determines most ribbon electronic properties and we are interested in how the edges affect the SOC in these structures. Study is performed for hydrogen terminated GNRs with the standard armchair and zigzag edges as well as the edges reconstructed in the way suggested by Koskinen et al [Phys. Rev. Lett. 101, 115502 (2009)], taking into account both the intrinsic and Rashba SOC.

71. Investigation local physic-mechanical properties of thin polymer layers using Atomic Force Microscopy

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We review the use of an Atomic Force Microscopy as a tool for investigating of the local dynamic physic-mechanical properties of the thin polymer layer in air environment. It is a method to study the properties of the polymers and biomaterials in nanometer scale. From the received results, we could obtain a better understanding of strongly interactions and receive some parameters of materials such as elastic, viscoelastic and the rheological property in nanoscale. The theoretical basic of the method to define these parameters is shown. Furthermore, the elastic modulus tip-sample interactions of the thin film Polivinilpiridina (PVP) prepared by Langmuir-Blodgett technology and the influences of the temperature and pressure on the properties of this film have been discussed in this paper.

72. Long range disorder effects on the heat capacity of two dimensional electron systems

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Broadening of Landau levels of two dimensional electron systems at low temperature and at high perpendicular magnetic fields causes perceptible variations in their interlevel and intralevel excitations as seen in their heat capacity. At a characteristic temperature, the interlevel excitations become negligible and the effect of a small broadening on the energy spectrum vanishes [1]. In this work, a long-

range disorder is considered. This can be modeled for the two dimensional electron gas via a Lorentzian density of states or a Gaussian density of states whose broadening is much larger than k_B T. The temperature of the heat capacity is derived at half-filled Landau levels or when the chemical potential is a constant. The heat capacity behavior of a system with a long-range disorder is compared to the case of impurity-free quantum Hall systems.

1] R. Gammag and C. Villagonzalo, The Interplay of Landau Level Broadening and Temperature on Two-Dimensional Electron Systems, Solid State Communications, 146, 487- 490 (2008)

73. Deposition of SnO2 and SnO2:F thin films by pneumatic sprayer deposition and study their optical and electrical properties

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Thin films of SnO2 and SnO2:F were deposited successfully by pneumatic sprayer deposition using dihydrate stannous chloride (SnCl2-2H2O) and ammonium fluoride (NH4F) as precursors. The substrate temperature was changed from 250 Â°C to 460 Â°C to determine the optimum temperature to deposit films. The films were characterized by X-ray diffraction (XRD) and SEM. Also, the optical and electrical properties studied by using UV-vis spectroscopy and Keithley multimeter respectively. The XRD pattern showed the presence of crystalline of SnO2 in the films deposited at temperature above 370oC while no XRD pick was found on the films deposited at temperature of 250oC. The films exhibited high transparent at the visible light area. Besides, the sheet resistance depends strongly on the content of NH4F in the precursor solution. The XRD peak positions tend to shift toward the high angle with the increase of NH4F content.

74. Ethanol gas sensor based on SnO2/ZnO and ZnO:Al films deposited by pneumatic sprayer deposition

Pham Van Vinh, Nguyen Van Hung , Bui Thi Hai and Dao Thi Hong Le

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Thin films of SnO2/ZnO and ZnO:Al for ethanol gas sensor were deposited successfully by pneumatic sprayer deposition. The films were characterized by X-ray diffraction (XRD) and SEM. Also, the ethanol sensitivity in deferent conditions was measured in order to determine the optimum working condition of sensor. The influence of doping concentration on structural and sensitivity properties of the films was studied in detail. The XRD pattern showed the presence of crystalline of SnO2 and ZnO in the SnO2/ZnO and ZnO:Al films. Although a considerable amount of impurity element was doped, no impurity phase was observed on ZnO:Al films while new phase of ZnO was found on SnO2/ZnO films. The grain size and sensitivity were varied depending on doping concentration.

75. DFT Study of Raman scattering in Fe-doped CaMnO3

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We present the Raman spectroscopy study of Fe-doped CaMnO3 magnetic perovksite compounds. The experimental results showed a rich set of scattering lines, many of which correspond to the forbidden and muliple phonons. The assignment was performed on basis of DFT calculation for optimized structure using PBE functionals and LANL2DZ basis set.

76. The Electronic Properties of MgO under High Pressure from Ab Initio Calculations

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MgO is not only one of the most abundant minerals in the Earth, especially in its lower mantle, but a material which is among the least polymorphic solids known, only one solid phase, with the NaCl structure type has been observed in experiments spanning pressures up to several hundreds GPa and temperatures up to several thousand

degrees Kelvin. Furthermore, it is known that atsufficiently high compression, all materials should become metallic, but MgO is very difficult to metallize. In this work, we present a first principles investigation of the electronic properties of MgO, the properties were obtained within density functional theory formalism thathas been proved to be very successful in the previous study for kinds of materials such as manganates [1] and polymers [2]. The electronic properties of the materials and the property evolution with pressure up to hundreds of GPa were studied and comparisons were made. It is found that the results are generally in good agreement with recent theoretical and experimental work.

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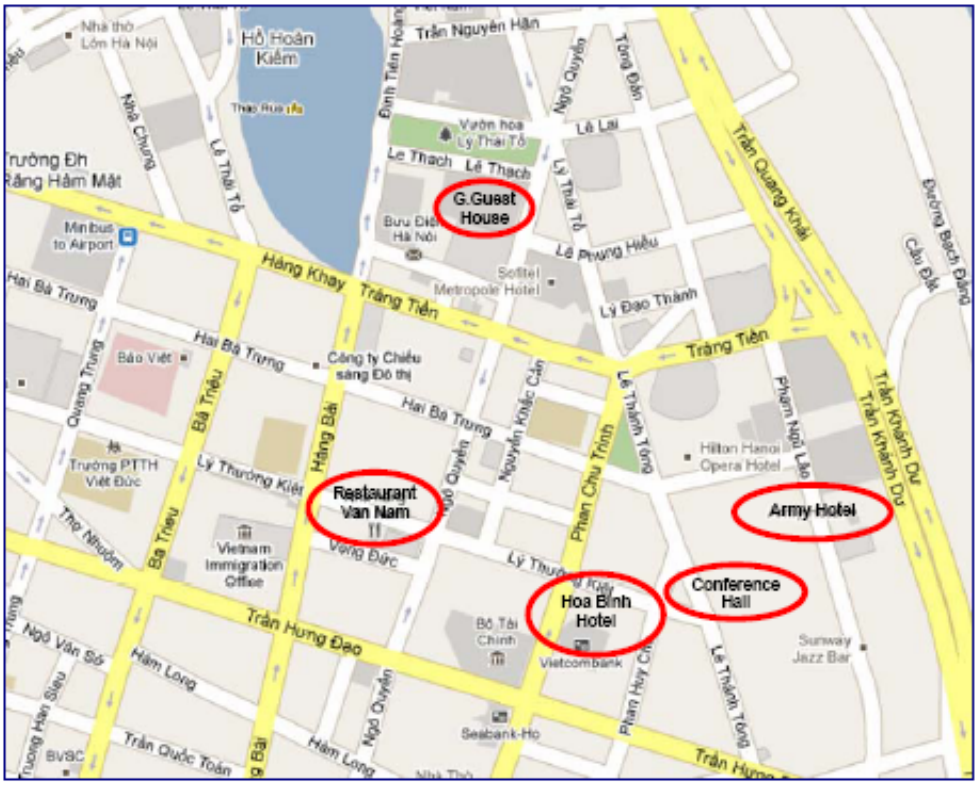
Author, Participant index

Map: Conference Hall, Hotel, Restaurant for APW 9



Banquet:

18h00, 13/12/2010
Hoa Binh Hotel
27 Ly Thuong Kiet, Hoan Kien, Ha Noi

Lunch:

12h25 – 14h00
Van Nam Restaurant
27b Ly Thuong Kiet, Hoan Kien, Ha Noi

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