The Schedule of the 5th International Conference on Condensed Matter Theory and Materials Computation

(July 10 – 15, 2006, Lanzhou, China)

第五届国际凝聚态理论与材料计算学会议(兰州 2006)

会议日程安排

July 10, ***Monday morning***

AM 8:00 – 8:10

Opening Remarks (Fa-Shen Li, Yu-Peng Wang, welcome)

Session 1 — Spintronics, magnetism

Chair: Xiang-Rong Wang

AM 8:10 - 8:30

Wave Packet View of the Dirac Electron

Qian Niu

(Department of Physics, University of Texas at Austin)

AM 8:30 - 8:50

Fingerprinting magnetization reversal in magnetic nanostructures

Kai Liu

(Physics Department, University of California at Davis, One Shields Ave, Davis, CA 95616, USA)

Chair: Qian Niu

AM 8:50 - 9:10

Magnetization reversal of Stoner particles by magnetic fields

Xiang-Rong Wang

(Physics Department, Hong Kong Univ. of Sci. & Technology, HongKong)

AM 9:10 - 9:30

Magnetism in Nanomagnets with Giant Magnetic Anisotropy

Bang-Gui Liu

（Institute of Physics, Chinese Academy of Sciences）

Abstract: We show that transition states during spin flips, besides inter-spin exchange and on-site anisotropy, are necessary to a complete description of monatomic spin chains, and study the dynamical spin system using kinetic Monte Carlo method based on transition-state theory. Using experimental parameters, we produce the experimental hysteresis loop at 10 K and show that there is no hysteresis loops at 45 K. There is a phase crossover from the long-range ferromagnetism at low temperature to disordered magnetic states at high temperature. The crossover temperature is a monotonously increasing function of the sweeping rate of changing magnetic field. Our theory explains the ferromagnetism of finite one-dimensional spin chains with large magnetic anisotropy. Since giant magnetic anisotropy has been realized experimentally, we use kinetic Monte Carlo method to study the spin dynamics of a nanomagnet that is made by putting a line of such adatoms on a thin metallic strip so that the fixed spins are coupled very weakly and a spin-polarized current can be injected into the strip. There is a magnetization hysteresis versus the current because of the giant anisotropy. The hysteresis loop is diminished exponentially with the temperature increasing. Our study shows that the magnetization can be controlled by injecting a spin-polarized current.

Chair: Kai Liu

AM 9:30 - 9:50

First-principles theory of quantum well resonance in double barrier magnetic tunnel junctions

Yan Wang,[1] X. F. Han[1], Zhong-Yi Lu[2] and X. G. Zhang[3]

[1]State Key Laboratory of Magnetism, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, PR China

[2] Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, PR China

[3]Computer Science and Mathematics Division, Oak Ridge National Laboratory,

Oak Ridge, Tennessee 37831, USA

Abstract: In this article we present a first-principles study of the Quantum well (QW) states in the symmetric epitaxial Fe(001)/MgO(001)/Fe(001)/MgO(001)/Fe(001) double barrier magnetic tunnel junction (DBMTJs). By including the Coulomb blockade energy due to the finite size islands of the Fe middle layer, we confirm that the oscillatory bias voltage dependence in the differential resistance observed in a recent experiment [1] originates from the QW resonances from the Δ_1 band of the Fe majority spin channel. By matching these QW states to the oscillations found in the experimental measurement, we find significant shifts in the QW resonances due to the Coulomb blockade effect arising from the finite size of the possibly discontinuous middle Fe layer. The scaling of the Fe island diameter with the thickness deduced from the Coulomb blockade energy shift is in good agreement with a previous AFM study [2].

Similarly to previous calculations [3, 4], the electrode layers of bulk iron and the middle iron film are fixed at the lattice constant of 2.86 Å and the MgO lattice constant is taken to be a factor of $\sqrt{2}$ larger than that of the iron. All calculations were performed using the layer Korringa-Kohn-Rostoker (Layer-KKR) implementation [5] of the local spin density approximation (LSDA) of the density functional theory. The self-consistent calculation is performed in the same manner as in Refs. 3-5. At the $\bar{\Gamma}$ point the $\Delta 1$ band is primarily *s*-character (angular momentum l = 0). In Fig. 1 (a), we show the calculated s-resolved partial density of states (DOS) at the $\bar{\Gamma}$ point within the central Fe layer in bcc Fe(001)/MgO/Fe9/MgO/Fe, with an 9 ML (monolayer) thickness of the Fe layer, compared with the s-partial DOS in bulk iron in Fig. 1 (b). The sharp spikes of the DOS in Fig. 1 (a) indicate the existence of majority spin QW states derived from the Δ_1 band of the Fe middle layer.

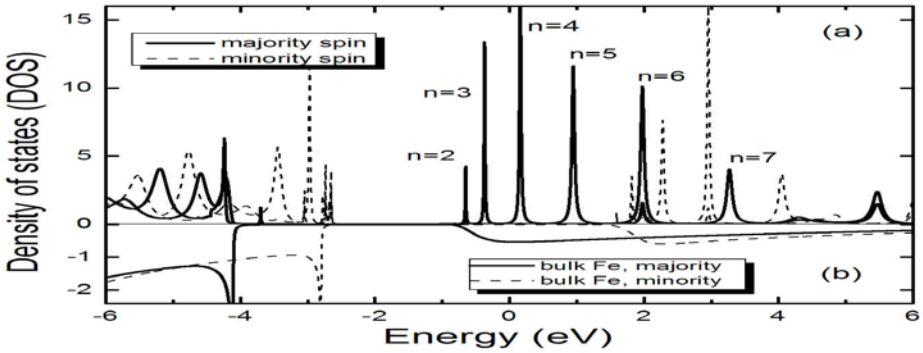

FIG. 1: *s*-resolved partial density of states at the $\bar{\Gamma}$ (k// = 0) point. Solid line, majority spin; dashed line, minority spin. (a) Within the central Fe layer in bcc Fe(001)/MgO/Fe9/MgO/Fe. (b) For bulk Fe. The Fermi energy is at 0 eV. *n* indicates the number of nodes in the wave function of majority spin QW states.

[1] T. Nozaki, N. Tezuka, and K. Inomata, *Phys. Rev. Lett.* **96**, 027208 (2006).
[2] E. Navarro, Y. Huttel, C. Clavero, A. Cebollada, and G. Armelles, *Phys. Rev. B* **69**, 224419 (2004).
[3] W.H. Butler, X.-G. Zhang, T.C. Schulthess, and J.M. MacLaren, *Phys. Rev. B* **63**, 054416 (2001).
[4] Zhong-Yi Lu, X.-G. Zhang, and Sokrates T. Pantelides, *Phys. Rev. Lett*. **94**, 207210 (2005).
[5] J.M. MacLaren, X.-G. Zhang, W.H. Butler, and Xindong Wang, *Phys. Rev. B* **59**, 5470 (1999).

AM 9:50 - 10:10

Magnetosubbands of semiconductor quantum wires with Rashba and Dresselhaus spin-orbit coupling

张胜利

(西安交通大学理学院)

Coffee break (AM10:10-10:20)

Chair: Guang-Ming Zhang

AM 10:20 - 10:40

有机纳米结构中的自旋极化输运

魏建华

（山东大学物理学院）

AM 10:40 - 11:00

SmTbCo 基垂直磁化多层膜的性能及层间耦合机理研究

苏深伟　余雪梅　王 翔

（北京航空航天大学电子信息工程学院）

Chair: 张胜利

AM 11:00 - 11:20

纳米磁性材料磁特性的 Monte Carlo 研究

黄志高

(福建师范大学物理系)

AM 11:20 – 11:40

非共线型磁性材料 CeRhIn5 的电子结构研究

胡文英

(中国科学院固体物理研究所)

AM 11:40 – 12:00

非晶态合金薄带及薄膜巨磁电阻抗效应定量计算模型与理论

鲍丙豪

(江苏大学机械工程学院)

July 10, *Monday afternoon*

Chair: Shi-Hai Dong

PM 2:00 –2:20

Effect of the normal metal layer on the differential conductance in ferromagnet / superconductor tunnel junctions

李 红

(中国石油大学（华东）化学化工学院)

PM 2:20 – 2:40

Stripe phase on a spin ladder with free boundaries

李 铭

(华南师范大学物理学院)

Session 2 — Quantum information and quantum computation in solid

Chair: Bang-Gui Liu

PM 2:40 - 3:00

Algebraic approach to position-dependent mass Schrodinger equation with a singular oscillator

Shi-Hai Dong

(Escuela Superior de Fisica y Matematica, Instituto Politecnico Nacional Edificio 9, Unidad Profesional Adolfo Lopez Mateos Mexico City, D.F. 07738, Mexico)

PM 3:00- 3:20

From quantum entanglement to classical phase transitions

Yu-Peng Wang

(Institute of Physics, Chinese Academy of Sciences)

PM 3:20 -3:40

Single qubit gates implemented through Spin-orbit Couplings

Zhongqin Yang

(Department of Physics, Fudan University)

Coffee break (PM3:40-3:50)

Session 3 — Nanoscale physics, surface physics, electronic structure,

semiconductor, low-dimensional systems, photonic crystal

Chair: 王雪华

PM 3:50 -4:10

Doping of Quantum Structures

Jianxin Zhong

(Oak Ridge National Laboratory, PO Box 2008, Oak Ridge, Tennessee 37831-6016
Department of Physics, Xiangtan University, Hunan 411105, China)
Email address: zhongjn@ornl.gov

Abstract: Recent breakthroughs in the growth of freestanding semiconductor quantum wires and quantum films have opened up great opportunities to revolutionize technologies in nanoscale electronics, optoelectronics, spintronics, and sensors. Doping, an essential element for manipulation of electronic transport in traditional semiconductor industry, is widely expected to play important role as well in control of transport properties in quantum structures. However, traditional theory of electronic disorder predicts that doping in one-dimensional and two-dimensional systems leads to carrier localization, limiting practical applications of doping in quantum structures because of poor carrier mobility. We proposed a novel concept, namely, segregative doping in quantum structures, to significantly increase carrier mobility [Zhong and Stocks, Nano Letters (2006)]. In our approach, distribution of dopants in a quantum structure is confined within a particular region in the structure so that the doped structure becomes a coupled system comprising a doped subsystem and a perfect crystalline subsystem. We showed that carrier mobility in a quantum wire or a quantum film with segregative doping exhibits rather counterintuitive behavior in the regime of heavy doping, namely, the larger the concentration of dopants the higher the carrier mobility

PM 4:10 – 4:30

Aluminum and iron bearing MgSiO3 under the deep Earth conditions

Feiwu Zhang

(Lab. of Crystallography, Department of Materials, ETH Honggerberg, HCI G512
Wolfgang-Pauli-Strasse 10 CH-8093 Zurich, Switzerlan)

Chair: Zhong-Qin Yang

PM 4:30 - 4:50

二维光子晶体中自发辐射的开关控制

王雪华

（中山大学理工学院）

PM 4:50 -5:10

Conductance Spectra of Metallic Carbon Nanotube Intramolecular Junctions

Wenxing Zhang[1], Wengang Lu[1], Hong Guo[2,3] and E. G. Wang[1,3]

1. Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences (CAS), Beijing 100080, China

2. Centre for the Physics of Materials and Department of Physics, McGill University, Montreal, Canada H3A2T8

3. International Center for Quantum Structures, CAS, Beijing 100080, China

A two-probe carbon nanotube (CNT) device is usually in the Metal-CNT-Metal configuration whose conductance sensitively depends on details of the Metal-CNT interfaces. When the metal leads are CNT themselves, namely for single wall CNT double intramolecular junctions in the form of $(n_1,m_1)/(n_0,m_0)/(n_1,m_1)$, due to rotational symmetry of the (n_0,m_0) section and quantum inference established between the two $(n_1,m_1)/(n_0,m_0)$ interfaces, rather universal behaviour of conductance spectra is found with respect to the relative rotational angle θ between the two (n_1,m_1) leads. In particular, we theoretically prove that the conductance spectra have either periodic dependences or no dependence at all on the angle θ. We further prove that when there is θ dependence, at most three different conductance spectra are possible for all allowed θ. Numerical results confirm the analytical prediction.

[1]. R. Saito, G. Dresselhaus, and M. S. Dresselhaus, Physical Properties of Carbon Nanotubes (Imperial College Press, London, 1995).

Chair: Jian-Xin Zhong

PM 5:10 - 5:30

Glycine on Cu surface

徐靖

(中国人民大学物理系)

PM 5:30 -5:50

Role of Lateral Alkyl Chains in Modulation of Molecular Structures on Metal Surfaces

Shixuan Du

（Beijing National Laboratory of Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences,Beijing 100080, China）

Abstract: We use low energy electron diffraction, scanning tunneling microscopy, first-principles density functional theory, and molecular mechanic calculations to analyze the adsorption and growth of quinacridone derivatives (QA) with alkyl chains of 4 and 16 carbon atoms on a Ag(110) substrate. Surprisingly, we find that the alkyl chains determine the orientation of the molecular overlayers. While the interaction of QA and the Ag substrate is primarily due to chemical bonding of oxygen to the silver substrate, determining the molecular orientation and preferred adsorption site, the intermolecular arrangement can be adjusted via the length of alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties.

July 11, *Tuesday morning*

Chair: Tao Xiang

AM 8:00 - 8:20

The theoretical study of atom diffusion process: from moving on a clean surface to climbing the hut

Yu Jia

(School of Physics and Engineering, Zhengzhou University, Zhengzhou 450052)

Abstract: Using the first principle and molecular dynamics method, we studied the diffusion behaviors of adatoms or clusters during the film growth process. Here two kind of cases are considered: (1) We first study a single adatom, such as Ge, Co and Ag, diffusion on the Ru(0001) surface, the stable and metastable adsorption sites are identified and the diffusion barriers along the all the diffusion paths are calculated. The results show that the hcp is the almost stable adsorption site for these adatoms and it is relatively easy for a adatom diffusion on Ru(0001) surface. (2) Another cases is that, for Al, or Cu huts which homoepitaxy growth along (110) direction, we found that the adatom, dimmer and trimer can easily diffuse upwards along the slope facet of (111) surface and across the edge to the top via simple exchange mechanism, while

the adatoms on the slope facet of (001) can also diffuse upwards and across the edge to the top through long exchange mechanism.

AM 8:20 - 8:40

纳米固体尺寸效应:原子配位缺陷理论及应用

孙长庆

(南洋理工大学, School EEE, NTU, Singapore)

Chair: 赵宏康

AM 8:40 –9:00

Accurate energy spectrum and spin-modulated conductance of finite width ring with Rashba spin-orbital coupling

J.W. Ding[1,2,3], R. Shen[2], and D.Y. Xing[2]

[1]Department of Physics, Xiangtan University, Xiangtan 411105, Hunan, China
[2]National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing, 210093 China
[3]Email address: jwding@xtu.edu.cn

Abstract: A more realistic model of finite width ring is built by considering a hard wall radial confinement. In the presence of the Rashba spin-orbital coupling and a flux, the energy spectrum is accurately obtained, using a nonperturbative treat with the azimuthal Hamiltonian, which shows a sample specific nature. Considering the inter-band coupling, the spin modulated conductance is also explored, depending on the mode number and the Fermi energy and thus on the applied bias and gate voltage, which was observed experimentally. A criterion for the inter-band mixing to be negligible is derived, which is useful for the designs and applications of mesoscopic ring devices.

AM 9:00 - 9:20

Electronic states of ErSi2 with and without vacancy by LSDA+U method

Zhongqin Yang

(Department of Physics, Fudan University)

Chair: Shi-Xuan Du

AM 9:20 – 9:40

Semi-classical molecular dynamics of nonlinear lattices

Tang Yi

(Department of Physics, Xiangtan University, Xiangtan 411105, Hunan, China)

Email address: tangyii@163.com

AM 9:40 – 10:00

Premelting of carbon nanotubes

Kaiwang Zhang

(Department of Physics, Xiangtan University, Xiangtan 411105, Hunan, China)

Email address: kwzhang@xtu.edu.cn

Coffee break (AM10:00-10:10)

Chair: Yu Jia

AM 10:10 –10:30

碳纳米管耦合系统中的发射噪声

赵宏康

(北京理工大学物理系)

AM 10:30 –10:50

纳米材料的量子从头计算

宋 炜

(北京大学物理学院凝聚态物理与材料物理研究所)

Chair: Wen-Gang Lu

AM 10:50 – 11:10

一维纳米材料量子从头计算

赖　林

(北京大学物理学院凝聚态物理与材料物理研究所)

AM 11:10 – 11:30

高压下过渡金属 **Fe** 的物性的计算研究

刘绍军

(北京师范大学物理系)

AM 11:30 –11:50

三端混杂系统热电输运性质的理论研究

陈志高

(福建师范大学物理系)

July 11, *Tuesday afternoon*

Chair:　魏建华

PM 2:00 –2:20

FePt 合金点缺陷研究

舒小林

(北京航空航天大学物理系)

PM 2:20 –2:40

含有拓扑缺陷的纳米碳管的输运性质

曾　晖

(湖南大学)

Chair:　陈志高

PM 2:40 –3:00

铁电纳米线光致发光性质

顾豪爽

(湖北大学物理学与电子技术学院)

PM 3:00 – 3:20

温控电护法大量制备碳纳米管

赵廷凯

(西安交通大学)

PM 3:20 – 3:40

Mutual catalyzed-birth of population and asset in their exchange-Driven growths

林振权

(温州大学物理系)

Coffee break (PM3:40-3:50)

Session 4 — Strongly correlated systems, high-Tc superconductivity, quantum Hall effect

Chair: 唐壁玉

PM 3:50 - 4:10

Effective two-band model of electron-doped superconductors

XIANG Tao, LUO Hong-Gang, and LIU Cheng-Shi

(Institute of Theoretical Physics and Interdisciplinary Center of Theoretical Studies, Chinese Academy of Sciences, Beijing 100080)

Abstract: We propose a weakly coupled two-band model with $d(x^2-y^2)$ pairing symmetry to account for the anomalous temperature dependence of superfluid density [1] and electronic Raman spectra [2] in electron-doped cuprate superconductors. This model gives a unified explanation to the presence of an upward curvature in superfluid density near Tc and a weak temperature dependence of superfluid density in low temperatures. Moreover, this model can also account for the *B*1*g* and *B*2*g* Raman spectra of electron-doped cuprate superconductors. It explains in a natural way why the *B*2*g* Raman peak occurs at a higher frequency than the *B*1*g* one at optimal doping, and how these two peaks change with doping in agreement with experiments. Our work suggests that the pairing in electron-doped cuprates has predominately $d(x^2-y^2)$ symmetry in the whole doping range.

[1] H. G. Luo and T. Xiang, Phys. Rev. Lett. 94, 027001 (2005).
[2] C. S. Liu, H. G. Luo, and T. Xiang, Phys. Rev. B 73, 174517 (2006).

PM 4:10 -4:30

Universal scaling behavior of c-axis resistivity in high temperature superconductors

LUO Hong-Gang[1], SU Yue-Hua[2], and XIANG Tao[1]

[1] *Institute of Theoretical Physics and Interdisciplinary Center of Theoretical Studies, Chinese Academy of Sciences, 100080 Beijing*

[2] *Center for Advanced Studies, Tsinghua University, Beijing 100084, China*

Abstract: We propose and show that the *c*-axis transport in high-temperature superconductors is controlled by the pseudogap energy and the *c*-axis resistivity satisfies a universal scaling law in the pseudogap phase. We derived approximately a scaling function for the *c*-axis resistivity and found that it fits well with the experimental data of multilayer cuprates such as $Bi_2Sr_2CaCu_2O_{8+\delta}$, $Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$, and $YBa_2Cu_3O_{7-\delta}$. For the single-layer cuprates, the c-axis resistivity shows a similar scaling behavior but the scaling function needs to be modified. Our works reveals the physical origin of the semiconductor-like behavior of the *c*-axis resistivity and suggests that the *c*-axis hopping is predominantly coherent.

[1] Y. H. Su, H. G. Luo and T. Xiang, Phys. Rev. B, 134510 (2006).

Chair: Hong-Gang Luo

PM 4:30 - 4:50

其他量子霍尔效应的协变基态

孙令鹏

（紫金山天文台）

PM 4:50 -5:10

NiO 的高压行为：强关联效应的影响

唐壁玉

(湘潭大学物理学院)

Session 5 — Bose-Einstein condensation, supersolid, quantum phase transition, statistical physics

Chair: 刘杰

PM 5:10 – 5:30

Spin in nematic phase of spin one cold boson on optical lattices

Guang-Ming Zhang

(Tsinghua Uinversity)

PM 5:30 – 5:50

全光型量子简并气体的实现与研究

印建平

(华东师范大学)

July 12, *Wednesday morning*

Chair: 印建平

AM 8:00 – 8:20

BEC 不稳定性研究

刘杰

(北京应用物理与计算数学研究所)

AM 8:20 –8:40

Ground-state properties of 1D trapped Bose gases

Shu Chen

(Institute of physics, Chinese Academy of Sciences)

Chair: Shu Chen

AM 8: 40 –9:00

BEC 中涡旋对的动力学研究

傅立斌

(北京应用物理与计算数学研究所)

AM 9:00 – 9:20

Nonlinear waves in Bose-Einstein Condensate

段文山

(西北师范大学物理与电子工程学院)

Chair: 段文山

AM 9:20 – 9:40

Dynamics of Bose-Einstein Condensates near Feshbach Resonance

Wu-Ming Liu (刘伍明)

(Institute of Physics, Chinese Academy of Sciences)

AM 9:40 – 10:00

双组份 BEC 中集体行为的研究

薛具奎

(西北师范大学物理与电子工程学院)

Coffee break (AM10:00-10:10)

Chair:　薛具奎

AM 10:10 – 10:30

First principles calculation of structural, thermodynamic properties and phase transition of lighter alkali-hydrides

Wen Yu [1,2] and Changqing Jin[1]

[1]*Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, People's Republic of China*

[2]*Physics Department, University of Science and Technology, Beijing, Beijing 100083, People's Republic of China*

Abstract: The structural, thermodynamic properties and phase transition of lighter alkali-hydrides (LiH, LiD and NaH) have been calculated by first principles density functional theory (DFT) and density functional perturbation theory (DFPT) with LDA and GGA exchange correlation functionals in the framework of quasiharmonic approximation (QHA). We found it is essential to include explicitly the semi-core electrons in the valence states of the alkali metals in order to make our calculation results comparable to the available experimental data. The calculated phonon dispersion curves, thermodynamic properties (thermal expansion coefficients, constant volume and constant pressure heat capacities, vibrational entropy etc.), room-temperature equation of states and *B*1-*B*2 phase transition pressures are all in good agreement with experiments.

AM 10:30 –10:50

自旋量子制冷循环

何济洲　梁红妮

（南昌大学物理系）

AM 10:50 – 11:10

非局域 Sun-Guo-Grant 方程的自洽模耦合理论

唐 刚

（中国矿业大学理学院，江苏徐州）

Session 6 - Soft condensed matter, polymers, biophysics

Chair: 邵 彬

AM 11:10 - 11:30

First-principles and Its Applications in Polymer Materials

郑 广

(中国地质大学(武汉)数学与物理学院)

AM 11:30 - 11:50

Structure and Metallization in GeH_4 under Pressure

Li Zhi, Yu Wen, Jin Changqing

(National lab for Condensed Matter Physics, Institute of Physics , CAS,

Beijing 100080)

Abstract: It has been shown that silane needs lower pressure to be metallized than hydrogen and undergoes phase transitions with sixfold- and eightfold- coordinated Si-H cluster appearing above 25GPa. Germane should have even positive metallization response under pressure. Using the first principle calculation, we calculated some possible structures and get their pressures at which they are metallized. It is found that GeH_4 is easier to be metallized than SiH_4. The lowest pressure to metallize GeH_4 is about 23Gpa .We also get the most stable structure under high pressure .

AM 11:50 - 12:10

淀粉样肽聚集的全原子分子动力学模拟

韦广红

(复旦大学物理系)

July 12, *Wednesday afternoon*

Chair: 韦广红

PM 2:20 - 2:40

氢键系统中的二分量扭结

成元发

(湖北大学物理学与电子技术学院)

PM 2:40 - 3:00

分子器件的光学性能研究

王磊

(湖南大学应用物理系)

Chair: 何济洲

PM 3:00 - 3:20

Density Functional Study on the Possibility of Synthesizing the Derivatives of the Nonclassical Four-Membered Ring Fullerene C_{62}

邓开明

(南京理工大学应用物理系)

PM 3:20 - 3:40

Structure of adsorbed polymers on a colloid particle

严大东

(中国科学院化学研究所)

PM 3:40 – 3:50

Concluding Remarks (Yu Jia, Yu-Peng Wang, welcome 6th CMT & MC conference)