

第一届国际凝聚态理论与材料计算学会议

第二轮通知

由中国科学院物理所凝聚态理论与材料计算研究室和山东大学威海分校举办的第一届国际凝聚态理论与材料计算学会议定于 2002 年 7 月 10-15 日在山东大学威海分校召开。

大会将对以下的问题做专题性的特邀报告。

(1). 凝聚态物理领域的最新进展:

- A. 强关联电子系统
- B. 高温超导理论
- C. 量子霍尔效应理论
- D. 纳米材料
- E. 磁学理论
- F. 表面和界面
- G. 半导体理论
- H. 低维凝聚态物理
- I. 介观物理
- J. 软凝聚态物质

(2). 材料计算学的最新进展:

- A. 基于第一原理的计算
- B. 蒙特卡罗模拟计算
- C. 基于分子动力学的模拟计算
- D. 密度泛函理论

注意事项:

1. 会议地点:

山东省威海市山东大学威海分校

2. 会议日期:

2002 年 7 月 10-15 日

3. 费用问题:

- A. 本次会议没有注册费
- B. 境内的专家会议费用自理
- C. 境外的专家的本地费用由会议主办方负责

4. 联系方式:

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5. 住宿:

九九大酒店（三星级宾馆）
标准间： 210 元/间*夜
酒店地址： 威海市高新技术开发区，鞍山路北首1号
（注：酒店到校园大约十分钟路程）
宾馆须包房提前预定。

6. 乘车路线：

A: 火车

B: 飞机

附录：

第一届国际凝聚态物理与材料计算学会议报告日程表。

2002 年 7 月 10-15 日，
威海, 山东, 中国。

会议日程安排

July 10 *Monday Morning*

Session 1, Chair: Yu-Peng Wang, Siu-Tat Chui

AM 8:00-8:50

Qian Niu (Texas Univ.)

Title: Quantum Step Heights in Hysteresis Loops of Molecular Magnets

AM 8:50 - 9:40

Zhen-Yu Zhang (Oak Ridge Nat. Lab.)

Title: Multiscale Study of Quantum Dot Formation in Heteroepitaxy:
From First-Principles Calculations to Continuum Elasticity Theory

Coffee Break (AM 9:40-10:00)

Session 2, Chair: Siu-Tat Chui

AM 10:00-10:50

Xi-Cheng Xie (Oklahoma State Univ.)

Title: Spin Polaron and In-plane Magnetic Field Effect in 2D
Metal-Insulator Transition

Abstract: For a two-dimensional electron system at low densities, there may exist a phase transition from the spin unpolarized to the fully polarized liquid state. A novel type of excitation, called spin polaron excitation, may form near the transition. The excitation causes the spatial inhomogeneous structure consisted of the unpolarized and the polarized regions with different local conductivities. Thus, the 2D metal-insulation transition can be understood as a semi-classical percolation transition. Within the picture, the observed energy gap is shown to be the energy needed to fully polarize electrons, and the in-plane magnetic field effect can be readily addressed. We find that the theory fits reasonably well with the experimental findings in p-GaAs/AlGaAs systems, where the disorder effect is less important.

AM 10:50-11:40

Guang-Shan Tian (Peking Univ.)

Title: Some Rigorous Results on the Strongly Correlated Electron
Systems by the Spin-reflection-positivity Method.

Abstract: In this talk, we shall briefly review some results on the strongly correlated electron systems, derived recently by applying Lieb's spin-reflection-positivity method. To explain the basic ideas of this method to a wide audience, we emphasize the important role played by Marshall's rule in studying the many-body systems.

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会议日程安排

July 10 *Monday Afternoon*

Session 3, Chair: Zhen-Yu Zhang

PM 2:00-2:50

Tao Xiang (ITP, CAS)

Title: Filter effect and the STM spectrum of high temperature superconductors

15:00-16:00

Shi-Ping Feng (Beijing Normal Univ.)

Title: Unusual physical properties in copper oxide materials: from
ladder to two-dimension

16:00-17:00

Guang-Ming Zhang (Tsinghua Univ.)

Title: Re-examine quantum spin 1/2 Heisenber antiferromagnets

17:00-18:00

Bang-Gui Liu (IOP, CAS)

Title: First-principle study of the half-metallic ferromagnetism



会议日程安排

July 11

Chairman: Guang-Shan Tian, Qian Niu

8:00-9:00

Siu-Tat Chui (Delaware Univ.)

Title: Realization of an Ultra-high Magnetic Field on a Nanoscale

9:00-10:00

Hong Guo (McGill Univ.)

Title: Theory and Numerics of Molecular Electronics

Abstract: We report a new ab initio technique for modeling nonequilibrium charge transport in molecular scale nanoelectronic devices. This technique is based on carrying out density functional theory (DFT) self-consistent analysis within the Keldysh nonequilibrium Green's function (NEGF) formalism. The NEGF-DFT technique overcomes several difficulties of doing first principles modeling of open molecular quantum coherent conductors at nonequilibrium. We report analysis of nonequilibrium electron transport in single molecule field effect transistors and diodes, molecular and atomic wire, as well as molecular tunnel junctions.

10:00-11:00

Xiang-Rong Wang (HongKong Sci. Techn. Univ.)

Title: Anti-resonance scattering at defect levels in the quantum conductance of a one-dimensional system

Abstract: For the ballistic quantum transport, the conductance of each channel is quantized to a value of $2e^2/h$. In the presence of defects, electrons will be scattered such that the conductance will deviate from the values of the quantized conductance. We show that an anti-resonance scattering can occur when an extra defect level is introduced into a conduction band. At the anti-resonance scattering, exact one quantum conductance of a one-dimensional wire disappears, in good agreement with ab initio calculations. The conductance takes a non-zero value when the Fermi energy is away from the anti-resonance scattering.

11:00-12:00

Hai-Qing Lin (HongKong Chinese Univ.)

Title: Quantum Monte Carlo Simulation on Parallel Machine

会议日程安排

July 11

Chairman: Shi-Ping Feng, Xi-Cheng Xie

14:00-15:00

Xiao-Qun Wang (ITP, CAS)

Title: Magnetic field
effects on Copper Benzoate: A Henseiberg antiferromagnetic
chain with Dzaloshiskii-Moriya interaction

15:00-16:00

Chang-Qin Wu (Fudan Univ.)

Title: Bond Order Wave in One Dimension

16:00-17:00

Yu-Liang Liu (Tsinghua Univ.)

Title: Eigen-functional theory and its application on quantum
many-particle systems

17:00-18:00

Zhao-Hua Cheng (IOP, CAS)

Title: Mossbauer spectroscopy and its application in Condensed Matter Physics



会议日程安排

July 12

Chairman: Tao Xiang, Hong Guo

8:00-9:00

Zi-Dan Wang (Hongkong Univ.)

Title:

9:00-10:00

Shi-Jie Xie (Shandong Univ.)

Title:

10:00-11:00

Xin-Gao Gong (Fudan Univ.)

Title:

11:00-12:00

Hong Chen (Tongji Univ.)

Title:

会议日程安排

July 12

Chairman:

14:00-15:00

Shun-Qing Shen (HongKong Univ.)

Title: Spin current in ferromagnetic metals and semiconductors

Abstract: We propose a microscopic theory to describe the exchange interaction between spin current and the spin torque in a system with strong Hund's rule coupling. Possible relevance to spintronics is discussed.

15:00-16:00

Wen-Jian Liu (Peking Univ.)

Title: "The Beijing relativistic density functional program package (BDF): a brief review and outlook"

16:00-17:00

Gang Sun (IOP, CAS)

Title: Optimization of the basis function in the full waveform inversion

17:00-18:00

Xin-Zhong Yan (IOP, CAS)

Title: Pairing fluctuation effect in d-wave superconductivity

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会议日程安排

July 13

Chairman: Guang-Ming Zhang, Zi-Dan Wang

8:00-9:00

En-Geng Wang (IOP, CAS)

Title: Atomic-scale study of surface based nanostructures:
Formation and Stability

9:00-10:00

Zheng-Yu Weng (Tsinghua Univ.)

Title:

10:00-11:00

Jian-Hua Wei (Shandong Univ.)

Title:

11:00-12:00

You-Quan Li (Zhejiang Univ.)

Title: On models with high rank symmetries in condensed matter physics



会议日程安排

July 13

Chairman:

14:00-15:00

Zhi-Dong Zhang (IMR, CAS)

Title: Quantum interference and exchange coupling in double quantum wells

15:00-16:00

Guo-Xiang Huang (East China Normal Univ.)

Title: Solitons in Bose-Einstein condensates

16:00-17:00

Yong-Li Ma (Fudan Univ.)

Title: Some properties of a trapped interacting Bose-Fermi gas mixture

17:00-18:00

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Title:

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会议日程安排

July 14

Chairman: Jian-Hua Wei, Xiang-Rong Wang

8:00-9:00

Sheng-Hao Han (Shandong Univ.)

Title:

9:00-10:00

Yu-Peng Wang (IOP, CAS)

Title:

10:00-11:00

Fu-Xiang Han (Dalian Sci. Techn.Univ.)

Title: Constrained Path Monte Carlo Study of Two-Layer Hubbard Model

11:00-12:00

Jing Shi (Wuhan Univ.)

Title: Critical behavior of Peierls Transition and Magnetic Quantum
Transport for Charge-Density-Wave Conductors



会议日程安排

July 15

Chairman: Sheng-Hao Han, Hai-Qing Lin

8:00-9:00

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9:00-10:00

Jin-Ming Dong (Nanjing Univ.)

Title:

10:00-11:00

Hang Zheng (Shanghai Jitong Univ.)

Title:

11:00-12:00

Wu-Ming Liu (IOP, CAS)

Title:

