CROUCHER FOUNDATION - ADVANCED STUDY INSTITUTE (ASI) ON

Frontiers in Computational Methods and Their Applications in Physical Sciences

Program

December 6 (Tuesday)

Registration: Room G25, Ground Floor, Science Centre North Block

December 7 (Wednesday)

Venue: L3, Science Centre

8:00 am Bus to workshop venue (assemble in hotel lobby)

8:30 am Light breakfast

Opening and Overviews

Session Chair: H. Q. Lin

9:00 am **K. Young** and **H. Q. Lin**: Opening

9:30 am **D. P. Landau**: Overview of Current Status in Simulation of Classical Systems

10:30 am Tea break; registration

11:00 am **R. Car**: Overview of Current Status in Simulation of Quantum Systems

12:00 pm Lunch; discussions; e-mail; registration

Topic: First Principles Calculations

Session Chair: D. S. Wang

2:00 pm **S. G. Louie**: First Principles Ground- and Excited-State Calculations: DFT, GW and Beyond

3:00 pm **R. Car**: Exploring DFT Potential Energy Surfaces: String and Metadynamics Approaches

4:00 pm Tea break

Session Chair: Q. Q. Zheng

4:30 pm **J. Tse**: A Perspective on the Crystal Structures of High Pressure Elements and Their Properties

5:15 pm **G. H. Chen**: First-principles Method for Open System

12:00 pm - 6:00 pm Poster Presentation (*Chair: Z. F. Liu*): *Ab initio Methods* [display for 2 days]

6:00 pm & 7:00 pm Bus to hotel

Note 1: "Light breakfast" refers to cakes, sandwich, and drinks
Note 2: "6:00 pm & 7:00 pm bus to hotel" means that the first bus leaves 6:00 pm, while the second one leaves 7:00 pm for people who prefer to dinning at the University
Note 3: for people who leave Hong Kong on December 14, we will arrange tour, shopping, etc., upon request. Accommodation is covered by us.

December 8 (Thursday)

Venue: L3, Science Centre or Room 707, Mong Man Wai Building

8:00 am Bus to workshop venue (assemble in hotel lobby)

8:30 am Light breakfast

Topic: Many-body Systems

Session Chair: S. P. Feng

9:00 am **D. M. Ceperley**: Quantum Monte Carlo Methods for Many-Fermion Continuum Systems in their Ground State

10:20 am Tea break

10:40 am **J. E. Gubernatis:** Quantum Monte Carlo for Electrons on a Lattice: Introduction and Methods

12:00 pm Lunch; discussions; e-mail

Topic: First Principles Calculations

Session Chair: Z. F. Liu

2:00 pm **S. G. Louie**: Quasiparticle Excitations and Optical Response of Bulk and Reduced-Dimensional Systems

3:00 pm **C. T. Chan**: Applying Electronic Structure Techniques to Photonic Calculation

3:30 pm Tea break

Session Chair: C. T. Chan

3:50 pm **Z. Fang**: First-principles Studies for the Anomalous Hall Effect and Spin Hall Effect

4:20 pm **G. Y. Guo**: Ab initio Calculations as a Tool for Discovery: Charge-orbital Ordering and Verwey Transition in Magnetite

4:50 pm **J. L. Yang**: First-principles Studies of BN Nanotubes

5:20 pm **H. Sun**: Ideal Strengths of Super-Hard Materials

9:00 am - 6:00 pm Poster Presentation (*Chair: Z. F. Liu*): *Ab initio Methods* (continues)

6:00 pm & 7:00 pm Bus to hotel

December 9 (Friday)

Venue: L3, Science Centre

8:00 am Bus to workshop venue (assemble in hotel lobby)

8:30 am Light breakfast

Topic: First Principles Calculations and Classical Monte Carlo

Session Chair: G. H. Chen

9:00 am **R. Car**: First Principles Molecular Dynamics: Applications to Water

9:50 am **S. G. Louie**: Deriving Insights from Computation: Molecular Electronics to Self-trapped Excitons

10:40 am Tea break

Session Chair: J. S. Wang

11:00 am **D. P. Landau**: Dynamic Scaling of Surface Growth in Simple Lattice Models

12:00 pm Lunch; discussions; e-mail

Topic: Computational Studies of Macromolecules

Session Chair: L. H. Tang

2:00 pm **Y. Duan**: Physics-based All-atom Simulations of Protein Folding and Aggregation

2:30 pm **L. H. Lai**: The Metabolic Network of Arachidonic Acid and Implications for Drug Design

3:00 pm **Q. Quyang**: The Cell-cycle Dynamics of the Budding Yeast

3:30 pm Tea Break

Session Chair: Z. Zeng

3:50 pm **E. Wang**: A Molecular Picture of Water Solid Interaction

4:20 pm **X. C. Zeng**: Water, Ice, and Bubble at Nanoscales

4:50 pm **X. G. Gong**: Constant Pressure MD Method and Its Application to Nano-cluster and Nano-tubes

5:20 pm **Z. F. Liu**: Links between Electron Microsolvation and Size Dependent Reactivity in Hydrated Mg^+ and Na Clusters

6:00 pm & 7:00 pm Bus to hotel

December 10 (Saturday)

Venue: L5, Science Centre

8:00 am Bus to workshop venue (assemble in hotel lobby)

8:30 am Light breakfast

Topic: Quantum Many-body Systems and Quantum Computing

Session Chair: X. C. Xie

9:00 am **D. M .Ceperley**: Path Integral Methods for Bosonic Superfluids

10:00 am Tea break

Session Chair: Y. D. Zhang

10:20 am **A. C. C. Yao**: Quantum Algorithms

12:00 pm Lunch; discussions; e-mail

Topic: Simulation of Classical Systems

Session Chair: E. G. Wang

2:00 pm **D. P. Landau**: The Search for Spin Waves in Iron above Tc: Spin Dynamics Simulations

3:00 pm **B. Zheng**: Monte Carlo Simulations of Phase Transitions - From Equilibrium to Non-equilibrium State

3:30 pm Tea break

Session Chair: Y. P. Wang

3:50 pm **J. S. Wang**: Worm Algorithms

4:20 pm **L. H. Tang**: Multicanonical Methods Applied to 2D XY Models

9:00 am - 5:00 pm Poster Presentation (*Chair: H. Q. Lin*): *Many-body Systems and Quantum Information* [display for 2 days]

5:00 pm - 5:30 pm Photo taking

5:30 pm Bus to banquet

6:00 pm Banquet

December 11 (Sunday) **Sight-seeing Tour**

December 12 (Monday)

Venue: L3, Science Centre

8:00 am Bus to workshop venue (assemble in hotel lobby)

8:30 am Light breakfast

Topic: "Exact Numerical Approach" to Quantum Many-body Systems

Session Chair: F. C. Zhang

9:00 am **T. K. Lee**: Superfluid and Supersolid Phases in Spin-dimer Model

9:30 am **P. Prelovsek**: Finite Temperature Dynamics of Strongly Correlated Electrons: Anomalous Properties of Cuprates

10:00 am **A. W. Sandvik**: Quantum Monte Carlo Simulation in the Valence Bond Basis

10:30 am Tea break

Session Chair: C. D. Gong

10:50 am **J. M. Dong**: Possible Tube-like Gold Clusters Au_{24} and Au_{26}

11:20 am **T. Xiang**: Recent Progress in Density Matrix Renormalization Group

11:50 am **X. Q. Wang**: Density Matrix Renormalization Group Method and Its Perspectives

12:20 pm Lunch; discussions; e-mail

Topic: Quantum Many-body Systems and Quantum Computing

Session Chair: T. Xiang

2:00 pm **J. E. Gubernatis**: Quantum Monte Carlo for Electrons on a Lattice: Applications and Issues

3:00 pm **G. Ortiz**: Simulating Physical Phenomena with a Quantum Computer

3:40 pm Tea break

Session Chair: J. E. Gubernatis

4:00 pm Panel Discussions on Future Developments and Summary

D. P. Landau (MC), **J. Tse** (Ab initio), **D. M. Ceperley** (QMC)

L. Yu: Summary

6:00pm & 7:00 pm Bus to Hotel

Poster Presentations

Topic: Ab initio Methods

K. W. Chan: Mg^+ in Different Solvation Clusters (NH_3 and CH_3OH)

L. W. Deng: First-principles Study of Orthorhombic Perovskites up to 120GPa and the Geophysical Implications

B. Gao: Size-dependent Charge Separation Reaction for Hydrated Sulfate di-anion Cluster, SO_4^{2-} $(H_2O)_n$, with n=3-7

H. Hong: Collective Synchronization in Locally Coupled Limit-cycle Oscillators

L. Lau: Oxidation Of Si(100) And Ge(100) Surface by Single Oxygen Molecule

H. Liu: Molecular Dynamics Simulations of Liquid Nitromethane under High Pressure and at High Temperature

J. W. Liu: Chemisorption of H_2 on Solid C_{60} under High Pressure

H. B. Su: Confinement and Catalysis in Formation of Tubular Fullerene Structures from Peapod Structures

L. F. Xu: Ab initio Study of Hygroscopic Properties of Borate Crystals

Z. Zeng: Magnetic and Spectral Properties of $NaxCoO_2$

L. Zhang: Equation of State of MgO up to 200GPa and 3000K: Combination of First-Principles Simulations and Experimental Data

Q. J. Zhang: Investigation of [2+2] Concerted Cycloaddition Mechanism for Unsaturated Hydrocarbon Chemisorption on Si(100)

Topic: Many-body Systems and Quantum Information

C. K. Chan: Spectral Methods and Their Applications

K. Chang: Rashba Spin-orbit Interaction and Spin Transport in Semiconductor Quantum Wells

X. J. Chen: How the Superconducting Transition Temperature Varies in Cuprate Superconductors

Y. G. Chen: Second- to First-order Transition in Two Coupled Antiferromagnetic Molecular Rings

R. Fan: Variational Monte Carlo Study of Na0.3CoO2.1.3H2O Superconductivity

Y. L. Liu: Universal Power-law Behavior of Local Electron Correlation Functions in the Falicov-Kimball Lattice Model

K. M. Tam: Functional Renormalization Group Analysis of the Half-filled One-dimensional Holstein-Hubbard model

Y. Q. Wang: Numerical Study of Magnetism in the Periodic Anderson Model

Y. Z. Zhang: Phase Transition in Checkerboard Lattice

L. J. Zou: Orbital Fluctuations & Orbital Ordering in Strongly Correlated Systems: Linearized Dynamical Mean-field Theory & Self-consistent-field Cluster Approach