In the past few years, we developed several new transition state searching methods (CBM, CBD, BP-CBD, DESW), and based on these methods, we designed a new global optimization method for potential energy surface (PES) search using the approximate normal mode (second derivatives), namely, stochastic surface walking (SSW) method \cite{J. Chem. Theory Comput. 2013, 9, 1838}. This method goes beyond the first derivatives, as most current algorithms do for PES search and at the same time does not compute accurate second derivatives, which are generally regarded to be essential for saddle point location. By adding bias potentials and performing local relaxation repeatedly, the SSW method can perturb smoothly the structure from one minimum to another following a random direction. The SSW method in combination with parallel replica exchange can be utilized for searching structure and predicting chemical reactions with a high efficiency. Using this method, we were able to identify the global minimum of short ranged Morse clusters, the carbon fullerene up to 100 atoms and Boron 40 cages based on classical potentials and first principles calculations. In this talk, I will give a few new examples of SSW method for structure searching, automated reaction prediction from solid phase transition to molecular reactions.

B14-06 Invited

Fast Motif Network Scheme for Crystal Structure Exploration of Silicate Cathodes for Li-Ion/Na-Ion Batteries

Shuqing Wu$^{1,2}$, Xin Zhao$^2$, Feng Zheng$^1$, Xiaobao Lv$^{2,3}$, Manh Cuong Nguyen$^1$, Cai-Zhuang Wang$^2$, Zijing Lin$^1$, Zi-zhong Zhu$^1$, and Kai-Ming Ho$^2$

$^1$Department of Physics, Xiamen University, Xiamen 361005, People’s Republic of China; $^2$Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA; $^3$Department of Physics, University of Science and Technology of China, Hefei, 230026, People’s Republic of China.

Research on the computational methods is the essence and soul of the development of computational condensed matter physics, and also a basis of independent software development. How to solve the “accuracy, speed, size” problems in the research on the computational methods has attracted great attention from the communities of physics, materials, energy and related fields. We recently proposed a search scheme based on motif network to study the crystal structures of the dilithium/disodium transition metal orthosilicates, i.e. $\text{A}_2\text{MsiO}_4$ ($\text{A} = \text{Li, Na}; \text{M} = \text{Mn, Fe, Co}$), which are promising cathode materials for Li-ion/Na-ion batteries. Using this fast and efficient scheme, the structures of all six combinations with $\text{A} = \text{Li or Na}$ and $\text{M} = \text{Mn, Fe or Co}$ were extensively explored in this work. All the structures of $\text{A}_2\text{MsiO}_4$ observed in the previous experiments can be found in our structure pool. In addition, existence of brand new structure can be expected in such systems. Some battery-related properties of several typical structures are also analyzed and discussed. The scheme proposed here can be easily extended to other similar systems and serve as a novel approach for extensive exploration of complex crystal structures.

B14-07

Pressure-dependent melting temperature of Xe

Ho Khac Hieu$^{1}$, Nguyen Thi Hoa$^2$

$^1$Institute of Research and Development, Duy Tan University, Vietnam
$^2$University of Transport and Communications, Vietnam

The Lindemann criterion was modified and combined with statistical moment method in quantum statistical mechanics to investigate the pressure effects on melting temperature of quantum solid Xeon. Numerical calculation of melting curve of Xeon has been performed up to pressure 50 GPa. Our results were compared with those of computational as well as experimental melting curve and showing the good and reasonable agreements. This approach gives us a relatively simple method for qualitatively calculating high-pressure melting curves of quantum solid Xeon. Moreover, it can be used to verify future experimental and theoretical works. This research proposes the potential of the combination of statistical moment method and the modified Lindemann criterion on predicting high-pressure melting of materials.
B15-01
Harnessing Network Properties to Manage Coupled Social-Ecological System
Hendrik Santoso Sugianto,*, Chung Ning Ying,2, Chew Lock Yue,*, Choy Heng Lay,3,4,*, Hendrik Santoso Sugianto
1School of Physical and Mathematical Sciences, Nanyang Technological University Singapore 637371, 2Complexity Institute, Nanyang Technological University, Singapore 639794, 3Department of Physics, National University of Singapore - Singapore 117542, 4Beijing-Hong Kong-Singapore Joint Centre for Nonlinear and Complex Systems, National University of Singapore, Singapore 119260, 5Yale-NUS College - 6 College Avenue East, Singapore 138614

Nowadays, the interaction between human and their environment is intense and inevitable. Our world is threatened by significant deterioration of forests, water resources, and biodiversity caused by human activities. One common problem is how rational and self-interested individual can cooperate to preserve their ecological resources. Recently Tavoni has introduced a model to study the establishment of cooperative behavior in coupled social-ecological systems through the ostracism mechanism. To make it more realistic, we have modified the model so that individual player makes discrete choice decision with the interaction constrained within certain network topology.

In this research we investigate the effect of several structural properties of a network that may affect the dynamics of coupled social-ecological system. For instance, by lowering the degree of the social network, our research has found a reduction in the width of the hysteresis curve. While a network with high connectivity is typically associated with a system that is robust with a resistance to change, it can however possess a high risk of sudden collapse. Interestingly, we found that a lowering of network degree can convert the critical transition from a sudden collapse to a more gradual change.

Network's topology also affects the regime shifts of such system. The hysteresis effect is stronger in scale-free network in comparison with random network. However both networks do not exhibit any community structure. It will be more realistic if we also investigate the effect of modularity on coupled social-ecological system, since in real society, people tend to live in groups. By investigating all these properties, we hope to understand the robustness and resilience in these systems with the aim of arriving at best management strategies to avert any unwanted regime shifts or collapses.

B15-02
Antiferromagnetic Ising model in an external field: critical behavior and convergence analysis using tomographic entropic sampling algorithm
Bruno Jeferson Lourenço,*, Ronald Dickman
Departamento de Física, ICEx, Universidade Federal de Minas Gerais – Brazil

One of the main issues concerning entropic simulation algorithms is the convergence of density of states (DOS) as the number of iterations increase. Using the tomographic entropic sampling (TES) algorithm, a flat-histogram simulation method, we perform convergence analysis of the DOS for the two-dimensional antiferromagnetic Ising model (IAF) in the presence of an external magnetic field on the square lattice. We note that bivariate simulation, as performed here, is a challenging task for entropic simulation methods. The TES algorithm uses a refinement parameter $f \sim t^a$ to update the estimate for the DOS after the $t$-th iteration, where $a$ is a real parameter. We verify that convergence occurs only for $0 < a \leq 1$, and $a=1$ yields the best rate of convergence. Using finite-size scaling analysis we estimate some critical points in the temperature-magnetic field plane; our estimates for the critical line allow us to test existing theoretical approximations. In addition, we study the phase transition along the critical line, acquiring good estimates for critical parameters $\beta/\nu$ and $\gamma/\nu$, related to critical values of the order parameter and staggered susceptibility, respectively.

B15-03 Invited
Bulk induced phase transition in driven diffusive systems
Yu-Qing Wang,*, Rui Jiang, Mao-Bin Hu
State Key Laboratory of Fire Science and School of Engineering Science, University of Science and Technology of China, Hefei 230026, China

This paper studies a weakly and asymmetrically coupled three-lane driven diffusive system. A non-monotonically changing density profile in the middle lane has been observed. When the extreme value of the density profile reaches $\rho = 0.5$, a bulk induced phase transition occurs which exhibits a shock and a continuously and smoothly decreasing density profile which crosses $\rho = 0.5$ upstream or downstream of the shock. The existence of double shocks has also been observed. A mean-field approach has been used to interpret the numerical results obtained by Monte Carlo simulations. The current minimization principle has excluded the occurrence of two or more bulk induced shocks in the general case of nonzero lane changing rates.

B15-04 Invited
Simulating spin models on GPU: An introduction
Martin Weigel
Applied Mathematics Research Centre, Coventry University, Coventry CV1 5FB, England

Over the last couple of years it has been realized that the vast computational power of graphics processing units (GPUs) could be harvested for purposes other than the video game industry. This power, which at least nominally exceeds that of current CPUs by large factors, results from the relative simplicity of the GPU architectures as compared to CPUs, combined with a large number of parallel processing units on a single chip. To benefit from this setup for general computing purposes, the problems at hand need to be prepared in a way to profit from the inherent parallelism and hierarchical structure of memory accesses.

In this overview lecture I discuss the performance potential for simulating spin models, such as the Ising or Heisenberg models as well as the Edwards-Anderson spin glass, on GPU as compared to conventional simulations on CPU. Different algorithms, including Metropolis [1,2] and cluster updates [3], as well as computational tricks such as multi-spin coding are taken into account.


B15-05
Applying Multi-GPU for Monte-Carlo numerical integration
L.Yu. Barash1,*, L.N. Shchur1,2
1Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia; 2Science Center in Chernogolovka, 142432 Chernogolovka, Russia

Monte-Carlo numerical integration has a number of important applications. Applying modern methods of calculations and massive parallelism can significantly improve performance of the integration. Monte-Carlo integration runs about 40-100 times faster on the GPU than on the CPU. Also demonstrated is a linear increase in performance of the Monte Carlo calculations with increasing the number of GPUs.