## Title:

Computational Materials and Modeling

## Abstract:

In recent years, the computational power of the ordinary user is increasing, and high performance computing is racing ahead. Great strides have been made toward combining computational, experimental and data science into a single integrated workflow, creating the framework for accelerating materials innovations. Thus, this is timely to set up the workshop on computational materials and modeling, which provides a forum to discuss how the increasing computational power can be used to enhance materials discovery and improve the understanding on complex material and device behaviors.

This workshop will bring together established experts and newcomers from academia, national laboratories, and industry to present the latest advances and discuss pressing challenges facing the computer-based modeling in materials research. One particular emphasis is on predictive modeling and simulations of novel energy materials based on quantum mechanical approaches, and critical experimental tests of such theoretical predictions. Another challenge is how to include advances in experimental characterization and data into computational materials design, such as temporally and spatially resolved in situ measurements. Alternatively, data analytics, such as inference and machine learning algorithms, are of great significance, which can be used to predict properties, either from large sets of experimental data or from modeling results.

## Scope and Topics:

This workshop is designed to invite authors to submit original manuscripts that demonstrate and explore current advances in all aspects of computational materials and modeling. The workshop solicits novel papers on a broad range of topics, including but not limited to:

- ✧ Fundamentals & Methodologies
- ✧ First-Principles Theory and Computation
- ✧ New Approaches in Materials Discovery
- ✧ Genetic algorithm for geometry optimization
- ✧ Molecular dynamics method for materials simulations
- ✧ Multiscale simulations and modeling
- ✧ Informatics and data analytics using simulation data

## Program Committee Chairs:

**Shiwei Lin**, Hainan University, China
linsw@hainu.edu.cn
http://www.hainu.edu.cn/stm/cailiaohuagong/20131015/10365869.shtml
Shiwei Lin received his Bachelor and Master degrees in Materials Science and Engineering at Tsinghua University. After that, he joined the Singapore-MIT Alliance program to obtain the second Master degree in Microelectronics. In September 2003, he joined the Microelectronics and Nanostructures (M&N) Group at the University of Manchester to start his PhD studies. In December 2006, he obtained the PhD degree working on the electronic characteristics of self-assembled InAs/GaAs quantum-dot structures. From September 2008 to September 2009, he worked in M&N group as Postdoc Research Associate and in Nano ePrint Ltd. Company as Device Engineer to investigate novel planar nano-scale electronic devices. Shiwei Lin joined Hainan University as an Associated Professor in 2007, and became Professor of Materials Science in 2008. He works mainly in the following research areas: metal-oxide semiconductor materials, flexible electronics, novel nanoelectronic devices, and atomic level modeling and computational materials science. He has authored or co-authored more than 110 peer-reviewed journal papers with more than 1300 citations.

**Cai-Zhuang Wang**, Ames Laboratory, US
wangcz@ameslab.gov
https://www.ameslab.gov/users/wangcz
Cai-Zhuang Wang, a physicist in the Laboratory's Division of Materials Science and Engineering, came to Ames Laboratory as a postdoctoral fellow in 1987. He joined the Laboratory's staff as an associate physicist in 1992. He received his Ph.D. in condensed matter physics at the International School for Advanced Studies in Trieste, Italy in 1986, and his bachelor's degree in physics at the University of Science and Technology of China in Hefei in 1982. Cai-Zhuang Wang has more than 320 refereed journal publications with citations more than 8600. He is famous for the significant advances in developing computation methods including tight-binding molecular dynamics for atomistic simulations, genetic algorithm for crystal and interface structure prediction, and Gutzwiller density functional theory for strongly correlated electron systems. In 2014, Cai-Zhuang Wang was named a Fellow of the American Physical Society (APS).

## Program Committee:

Cai-Zhuang Wang, Ames Laboratory, US
Kai-ming Ho, Ames Laboratory, US
Prof. Xingao Gong, Fudan University
Prof. Xuebin Chi, Computer Network Information Center, Chinese Academy of Sciences
Prof. Hai-Qing Lin, Beijing Computational Science Research Center

Shiwei Lin, Hainan University, China
Yunfeng Shi, Rensselaer Polytechnic Institute, US
Songyou Wang, Fudan University, China
Shunqing Wu, Xiamen University, China
Jun Xie, Hainan University