Title:

Computational physical and chemical properties of materials

Abstract:

The workshop “Computational physical and chemical properties of materials” is a new constituent in the 4th International Conference on Cloud Computing and Security (ICCCS 2018). Our goal is to provide the opportunities for the new frontiers in computer sciences applying in the computational physics, chemistry, and material science. It will be a good chance to meet and discuss with experts and scientists in various areas. We will provide a forum for researchers, academicians, engineers, industrial professionals, students and government officials discussing all the important issues in computational physics and chemistry, and materials science. The main purpose is to share new ideas and enjoying in-depth discussion within the computational disciplinary fields. All aspects of modern materials modelling are of interest, including quantum chemical methods, ab initio calculations, first-principles calculation, structural materials, properties of materials under electric and magnetic field, molecular dynamics simulation, optical properties and spectroscopy of materials, computational functional materials, quantum and classical Monte Carlo Simulation, nonlinear optics and all the others related to computational physical and chemical properties of materials. The workshop consists of oral and poster presentations. All the scientists, researchers and students from all over the world on the computational materials and the related are greatly welcome to join us.

Scope and Topics:

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

- ✧ Quantum chemical methods
- ✧ First-principles calculation
- ✧ Structural materials
- ✧ Properties of materials under electric/magnetic field
- ✧ Molecular dynamics simulation
- ✧ ab initio calculations
- ✧ Optical properties and spectroscopy of materials
- ✧ Computational functional materials
- ✧ Monte Carlo Simulation (quantum and classical)
- ✧ Nonlinear optics of materials
- ✧ All the others related to computational physical and chemical properties of materials

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Dr Zemin Ning conducts active research in genome informatics, specializing in sequence alignment and genome assembly. His main duties include developing algorithms and software tools for genome analysis at the Sanger Institute. Trained in Physics and Engineering, Dr Zemin Ning has been active in genome informatics for 16 years. After completing a PhD degree at Aston University and postdoc training at the Cavendish Laboratory, Cambridge University, he joined in the Sanger Institute in 1999 to pursue bioinformatics research. Over the past years, he and his colleagues in the group have developed a number of bioinformatics tools, which are widely appreciated by the genomics community. The group has also produced over 30 de novo assemblies from large animal and plant genomes, including Gorilla, Zebrafish, Tasmanian Devil, Bamboo and Miscanthus.

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Yuzhu Liu is Professor in the School of Physics and Optoelectronic Engineering, Nanjing University of Information Science and Technology. Along his career, he has published over 70 research papers on laser spectroscopy and molecular dynamics. His research interests include atmospheric optics, environmental optics, DFT calculation on degradation via electric field, DFT calculation on molecular spectroscopy and dissociation dynamics

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Yuanyuan Zhao is University Professor in the School of Physics and Optoelectronic Engineering, Nanjing University of Information Science and Technology. She has published over 10 research papers on theoretical condense matter physics, and she has experience on the GPU calculation as well. Her research interests include graphene, topological insulator, superconductor, topological superconductor, magnetism, first-principles calculations, and Monte Carlo calculations.

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