

Outstanding Professors in HPC Applications of ERA

Xingqiu Chen, he works as a professor of Institute of Metals, Chinese Academy of Science, and was elected One Hundred Person Project of the Chinese Academy of Science. His Research interests are Computational Materials Science and First-principles calculations, etc.

Haiping Fang, professor, is the director of Interfacial Water Division of Shanghai Institute of Applied Physics (SINAP), CAS. His Areas of Research are the interdisciplinary research of interfacial water, nano-biology and theoretical physics, especially the behavior of water at the nanoscale, its biological significance, and inspired nanoscale statistical physics. His works in the behavior of single file water chain, molecular-scale hydrophilicity, ratchet effect at nanoscale have been highlighted by Chinese Science Bulletin, Nature Nanotechnology, Nature Materials, New Scientist, Chemical World, Nature China, etc.

Liang Gao, professor in Astronomy, has mainly been developing state of art Cosmological simulations to study the large scale structure of the Universe, Galaxy formation and evolution as well as the nature of dark matter. Currently he and his team is developing a new Multi-Cores Cosmological N-body code based on the Intel Phi architecture.

Yiqin Gao, the director of the college of Chemistry and Molecular Engineering of Beijing University, Distinguished Professor of Yangtse River Scholar. He is doing research in the fields of theoretical/computational chemistry and biophysical chemistry.

Lixin He, professor, material science, he obtained his B.S. degree from the University of Science and Technology of China (USTC) in 1994, and Master degree in 1997. He studied the first-principles methods with Prof. David Vanderbilt at the Department of Physics and Astronomy of Rutgers University and obtained his Ph. D degree in 2003. From Sept. 2003 to Jan. 2006, Prof. He worked as a postdoctoral fellow at the Solid State Theory group in the National Renewable Energy Laboratory (NREL) with Dr. Alex Zunger, where he focused on the physical properties of semiconductor quantum dots. He then joined the Key Laboratory of Quantum Information, USTC as a faculty member. He was elected as IOP fellow (UK) in 2012. His major contributions are: (1) discovered and proved that in a 1D crystal the decay properties of Wannier functions and density matrices can be written as a power law decay times a exponential decay; (2) predicted that the InAs/InSb quantum dots have strongly correlated excitonic ground states, i.e. the electron-hole pairs can form spontaneously in these dots. He also worked on the physical properties of high dielectric, ferroelectric, multiferroic materials; the electronic structure of self-assembled

quantum dots, and the electron entanglement etc.

His research interests are: (1) develop the first-principles methods and apply them to study real materials; (2) study the electronic and optical properties of semiconductor quantum dots and their applications in quantum information and quantum computing.

http://lqcc.ustc.edu.cn/helx/helx_english.html

Jun Li, professor, chemistry, Tsinghua University, his research Interests are Quantum Inorganic Chemistry, Theoretical Actinide Chemistry, Computational Catalysis, Cluster Science, Computational Chemistry.

<http://www.junlilab.org/index.html>

Ligang Li, professor of Shanghai Astronomical Observatory, Chinese Academy of Sciences, uses Era to solve partial differential equations to study the fundamental mechanics of rotating fluid and fluid dynamics in the Earth and planetary interiors, such as planetary dynamo and mantle convection.

Lei Liu, Ph.D. supervisor, a professor of Institute of Biomedical Sciences in Fudan University, an associate director of Shanghai Center for Bioinformatics Technology, and a director of Department of Translational Medicine in Shanghai Public Health Clinical Center.

Experience: 1984-1988, Peking University, the School of Life Science, Bachelor degree major in Genetics. 1988-1991, Institute of Developmental Biology, Chinese Academy of Sciences, Master degree major in Developmental Biology. 1991-1997, University of Connecticut, Storrs, CT, Ph.D. degree major in Cell Biology. 1997-1999, Department of Computer Science and Engineering, University of Connecticut, Storrs, Connecticut, Postdoctoral Fellow. 1999-2007, the W. M. Keck Center for Comparative and Functional Genomics, the University of Illinois, Urbana, Illinois, Director of Bioinformatics. Since 2013, Institute of Biomedical Sciences, Fudan University, Professor, engaged in studies on biomedical informatics research, biomedical data integration and data mining, clinical decision support, personalized medicine, and achieved a series of innovative results, developed a series of medical health software system.

He had undertaken two projects from National 863 Programmes, and two projects from National Key Projects. He had published more than 60 research papers indexed by SCI, obtained 20 software copyright, and applied for six patents.

Jizhong Lou, Professor of Biophysics, combines computational, theoretical and single-molecule biophysics approaches to study how the conformations of biomolecules are regulated by external stimuli and characterize the mechanism of these conformational changes at the atomic level.

Shouqin Lü, associate professor, biomechanics, is interested in understanding the biomechanics and biophysics rules of important bioprocess in molecular and atomic level using experimental and computational methods.

Fei Sun, Professor of Structural Biology, Institute of Biophysics, Chinese Academy of Sciences, the research field of Dr. Sun's team is majorly related to structural biology. His team (<http://feilab.ibp.ac.cn>) combines cryo-electron microscopy (cryoEM) and X-ray crystallography as well as other biophysical and biochemical approaches to study the molecular architecture of biological systems. In the past seven years (2008-2014), they have got great achievements not only on the scientific merits but also on the construction of the infrastructure of cryoEM researches.

Bin Wang, professor in Atmospheric Sciences, focuses on numerical modeling of atmosphere including numerical weather prediction and climate simulation, decadal prediction and long-term projection. He and his group have developed several versions of the Grid-point Atmospheric Model of IAP LASG (GAMIL), whose coupled versions FGOALS-g1 and FGOALS-g2 (Flexible Global Ocean-Atmosphere-Land System, Versions g1 and g2) were one of the IPCC AR4 models and AR5 models,

respectively. In particular, FGOALS-g2 has been regarded as one of the best models in the world on ENSO simulations.

Weihua Wang, Professor, Institute of Physics, Leader of group of Formation, Physical Chinese Academy of Sciences Properties and Structure of Metastable Materials. His Research Interests are formation, microstructure, and physical properties of bulk multicomponent metallic glasses under high pressure and microgravity.

Yanting Wang, professor of the Institute of Theoretical Physics, Chinese Academy of Sciences. His main focus is the structural and dynamic properties and self-assembly processes of various kinds of soft matters as well as their microscopic mechanisms. Our current research interests include self-assembly of nanometals and peptides, structural and dynamic properties of ionic liquids and ionic liquid crystals, thermodynamics and statistical mechanics of soft matter, and coarse-graining methodology for molecular simulation.

Yujie Wei, Professor of State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences. His research interests include (a) Stable and unstable plastic deformation mechanisms in amorphous materials with different structural length scales, at different

temperature and loading rates. Propagation and multiplication of shear bands in amorphous solids; (b) Mechanical deformation behavior in nanocrystalline metals, thin films, nanointerconnects and ceramics, in particular to develop more faithful physical based understanding and modeling strategy for grain boundaries in nanocrystalline metals and ceramics; and develop methods on modeling the reliability of small-scale structures where mechanics and mass diffusion are coupled; and investigate the mechanical behavior in metals under the influence of diffusion, corrosion, and deformation. (c) Mechanical behavior in biosystems and biomaterials, the mechanical behavior of extra-cellular matrix, the strengthening and toughening mechanisms in bio-structured materials, dynamics of molecular bonds (d) Mechanics and deformation in hexagonal close-packed materials (hcp), lightweight metallic alloys and composite materials. An integrated research approach including experiments, theory development, continuum level computation, and atomistic scale simulation, is applied to those problems.

Jingfa Xiao, professor, Beijing Institute of Genomics, Chinese Academy of Sciences, genomics and bioinformatics, has done the work on comparative genomics analysis of Cassava (*M. esculenta*), pangenomics analysis of host-microbe interactions for pathogenic bacterium *S. suis* and *S. Paratyphi*, and development of new computational strategies for bacterial

pangenomics analysis. He uses Yuan Super Computing to integrate and analyze large-scale omics data.

Chao Yang, professor, Computer Science, is the director of the Peta/Exa-scale computing office in the Laboratory of Parallel Software and Computational Science at the Institute of Software, Chinese Academy of Sciences. His research interests include numerical analysis and modeling, large-scale scientific computing, and parallel numerical software.

Jinlong Yang, Professor of Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China. His current research topics are: (a)DFT and TDDFT Studies of Atomic Clusters (fullerenes, transition-metal oxide clusters,...); (b)STM Image and dI/dV Mapping Simulation; (c)Theoretical Studies on Nanotubes (adsorption,deformation,doping,...); (d)Transport Properties of Molecular Devices; (e)Electronic Structure of Novel Surfaces and Bulk Materials; (f)New Computational Methods and Codes. His research interests are: (a)Molecules, Clusters, Nanoparticles, Surfaces; (b)Theoretical and Computational Chemistry; (c)Computational Condensed Matter Physics and Material Physics.

Lei Yang, professor, director of the department of spallation target and the department of computational physics in Institute of Modern Physics, Chinese Academy of Sciences, visiting professor in Lanzhou University and Northwest Normal University.

2001 - 2003: Received a post-doctoral fellowship from Forschungszentrum Juelich. Research on nonlinear dynamics in fluid physics, mass-parallel computational method, nonlinear thermal transport phenomenon of low-dimensional system.

2003 - 2006: Group leader of Centre for Nonlinear and Complex System, Hong Kong Baptist University. Research on transport processes and complex system dynamics.

2006 - : Be selected as "100-Talent Programme" of CAS, start working in Institute of Modern Physics, CAS. Research on nonlinear transport processes, high power spallation target and GPU mass-parallel computational method.

Yongqiang Yu, Professor, Climate Modeling and Climate Change, is a lead principal investigator for the Earth System Model Development at the State Key Laboratory of Numerical Modeling for Atmospheric Sciences and Geophysical fluid Dynamics (LASG), Institute of Atmospheric Physics (IAP), Chinese Academy of Sciences(CAS). His group developed a global ocean model named as "LASG/IAP Climate system

Ocean Model” (LICOM), and a global coupled model named as “Flexible Global Ocean-Atmosphere-Land System” (FGOLAS), which had been applied in numerical simulation of anthropogenic climate change for the international Coupled Model Inter-Comparison Program (CMIP).

Zhi Zeng, Professor, Material Science, is a deputy director of the Institute of Solid State Physics, Chinese Academy of Science. Her research interests include magnetism, transportation properties, structural information under high pressure, strongly-correlated systems, multiscale computational methods. She is studying energy band structure and its control characteristics of materials using first-principles calculation. In her research, dynamical behaviors of materials were also studied using Molecular Dynamics simulation. Detailed information can be found at the following link: <http://english.issp.ac.cn/viewanlie2.asp?id=99&lanmu=>.

Linbo ZHANG, professor, Computational Mathematics and High Performance Computing. Zhang is deputy director of State Key Laboratory of Scientific and Engineering Computing of Chinese Academy of Sciences. He is co-author of China HPC TOP100 List. He wrote the parallel adaptive finite element toolbox PHG (Parallel Hierarchical Grid, http://lsec.cc.ac.cn/phg/index_en.htm) which provides fully parallel newest-vertex bisection based mesh adaptation algorithms for tetrahedral

meshes and can be used to develop scalable adaptive finite element applications.

Youliang Zhang, Professor, Institute of Rock and Soil Mechanics, Chinese Academy of Sciences, focuses on application of high performance computing in geotechnical engineering. Currently, his work mainly include the identification of multiple parameters in nonlinear constitutive model using asynchronous parallel particle swarm optimization and differential evolution algorithm, and the simulation of the whole process of rock masses failure using numerical simulation method combined with high performance computing technique.

Guangqing Zhou, Professor, Director of Information Center, Institute of Atmospheric Physics (IAP), Chinese Academy of Sciences. His research areas are development of ocean model and air-sea coupled models, short-term climate prediction, especially ENSO prediction, oceanic data assimilation and its application in short-term climate prediction and data management.

Lei Zhou, research fellow in the AVIC Computing Technique Research Institute. His research interests include high performance computing, aerodynamic analysis of aircraft, aero-elastic simulation.