第三届“凝聚物质的激发态”研讨会（线上会议）

The 3rd Workshop on Excited States in Condensed Matters (Online)
December 3rd, 2020

Training Session

Hefei-NAMD (8:00 - 8:30)
TDAP (8:30 - 9:00)

Session 1 (Chair Jin Zhao)

Hrvoje Petek (9:00 - 9:50)
Title: Non-Einsteinian Plasmonic Photoemission from Silver

Oleg Prezhdo (10:00 - 10:50)
Title: Ab Initio Quantum Dynamics in Modern Nanoscale Materials

Mohan Chen (11:00 - 11:50)
Title: Large-Scale First-Principles Methods: Recent Developments and Applications

Session 2 (Chair Sheng Meng)

Suhuai Wei (13:30 - 14:30)
Title: Band Structure Engineering and Doping Control of Transparent Conducting Materials

Jimin Zhao (14:30 - 15:30)
Title: Electron-phonon Coupling in Iron-based Superconductors and High Pressure Ultrafast Dynamics in Sr2IrO4

Xinguo Ren (15:30 - 16:30)
Title: Pushing the Limit of Electronic-structure Calculations with Numerical Atomic Orbitals

Huaixin Yang (16:30 - 17:30)
Title: Development and Application of UTEM in Material Science

Wentao Zhang (17:30 - 18:30)
Title: Ultrafast Nematic Electronic Phase Transition in FeSe

Short biography of the invited speakers:

Hrvoje Petek

Professor of Chemistry at the University of Pittsburgh. He vas born in Yugoslavia and received his degrees in Chemistry from MIT (BS; 1980) and U.C. Berkeley (PhD; 1985). From 1985 to 1993 he was first a postdoctoral fellow and a Research Associate at the Institute for Molecular Science in Okazaki, Japan. In 1993 he joined the Hitachi Advanced Research Laboratory as a Group Leader. In 2000 he joined the University of Pittsburgh, and concurrently consummated the Alexander von Humboldt Award at the Fritz Haber Institute in Berlin. His research interests span ultrafast spectroscopy and microscopy of solid-state materials and surfaces. He pioneered coherent multiphoton photoemission as a method for investigating coherent electron dynamics on the femtosecond temporal and nanometer spatial scales at semiconductor and metal surfaces. He received Chancellor's Distinguished Research Award from Pitt, 2019 Ahmed Zewail Award in Ultrafast Science, Luo Jia Visiting chair Professorship (Wuhan University), is a Fellow of the American Physical Society and American Association for the Advancement of Science, etc. Since 2006 he has been the Editor-in-Chief of Progress in Surface Science.

Oleg Prezhdo

Oleg V. Prezhdo obtained a Diploma in Theoretical Chemistry in 1991 from Kharkiv National University, Ukraine, under Anatoly Luzanov. He completed his Ph.D. with Peter Rossky at the University of Texas, Austin. After a postdoctoral fellowship with John Tully at Yale University, he joined the chemistry department at the University of Washington in 1998, achieving Associate and Full Professor in 2002 and 2005. In 2008, he was elected Fellow of the American Physical Society, and in 2010 was offered Senior Professorship at the University of Rochester. In 2014 he moved to the University of Southern California. He served as Senior Editor in multiple journals: in 2008-2020 for Journal of Physical Chemistry, in 2011-2019 for Journal of Physical Chemistry Letters, and in 2013-2019 for Surface Science Reports. Since 2020, he is Executive Editor for Journal of Physical Chemistry Letters. Recipient of multiple national and international awards, he held invited professorships in France, Germany, Spain, Ukraine, Japan, and China. His current h-index is 75. With over 400 papers and over 400 invited talks, Prezhdo's research interests range broadly from fundamental aspects of semiclassical physics and time-dependent density functional theory, to dynamics in nano-scale, condensed matter and biological systems.

Mohan Chen

Mohan Chen received his Ph.D. degree in physics at the University of Science and Technology of China in 2012. He was a postdoc in Mechanical and Aerospace Engineering at Princeton University from 2012 to 2016 before joining Department of Physics at Temple University as a postdoc in 2016. He joined the Center of Applied Physics and Technology at Peking University, Beijing, China, as an Assistant Professor in 2018. His research focuses on developing predictive computational algorithms within the framework of density functional theory, and their applications in materials sciences.

Xinguo Ren

Xinguo Ren obtained his PhD from University of Augsburg in Germany in 2006. From 2006 to 2012, he worked as a postdoc researcher at the Fritz Haber Institute of Max Planck Society in Berlin. In early 2013, he became a professor at University of Science and Technology of China in Hefei, and had worked there until 2019. He joined the Institute of Physics, Chinese Academy of Sciences as a faculty member In November, 2019. In 2015, Dr. Ren was appointed as the head of Max Planck Partner Group for Advanced Electronic-Structure Methods. Dr. Ren's research has been focused on (i) density-functional theory with advanced exchange-correlation functionals, especially those based on random phase approximation and beyond, (ii) Green's function theory for excited state calculations, and (iii) the development of computer software packages for large-scale ab initio calculations. Dr. Ren authored and coauthored more than 50 journal papers with over 5000 citations, and delivered more than 40 invited talks at international conferences and workshops. He received the IBM-Löwdin award from the Sanibel Symposium in 2011.

Suhuai Wei

Su-Huai Wei is a Chair Professor and Head of the Materials and Energy Division of the Beijing Computational Science Research Center (CSRC). He received his B.S. in Physics from Fudan University in 1981 and Ph.D. from the College of William and Mary in 1985. He joined the National Renewable Energy Laboratory (NREL) in 1985 and was a Laboratory Fellow and Manager of the Theoretical Materials Science Group before he joined the CSRC in 2015. His research is focused on developing electronic structure theory of materials, especially for semiconductors and energy related materials and their related applications. He has published more than 500 papers in leading scientific journals, including more than 70 in Physical Review Letters with more than 56,000 citations and an H index > 118. He is a Fellow of both of the American Physical Society and the Materials Research Society.

Huaixin Yang

Huaixin Yang is a full professor of Institute of Physics, CAS. Her currently research interest is the development and application of Ultrafast Electron Transmission Microscopy (UTEM). UTEM combines the ultrafast pump-probe method with TEM, therefore, it is a powerful experimental tool for the investigation of ultrafast dynamics at the nanoscale, combining a femtosecond temporal resolution with vast capabilities in imaging, diffraction, and spectroscopy. UTEM has introduced significant opportunities to directly visualize the atomic, electronic, and magnetic structural dynamics of materials.

Wentao Zhang

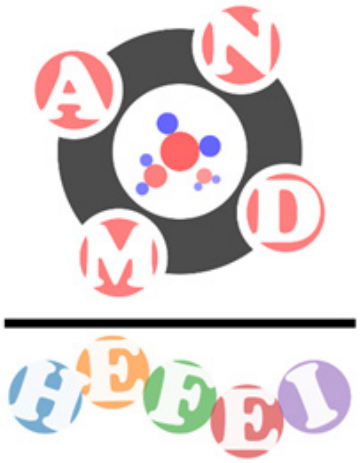
Wentao Zhang is from the School of Physics and Astronomy, Shanghai Jiao Tong University (SJTU), focusing on the study of ultrafast electronic and lattice dynamics in quantum materials by experiments. The technique I'm using time- and angle-resolved photoemission spectroscopy (trARPES) and MeV ultrafast electron diffraction. He is interested in pump-induced phase transition or even the phase emergence in strongly correlated materials.

Jimin Zhao

Jimin Zhao is a full professor at Institute of Physics, CAS. His research interest is ultrafast spectroscopy and dynamics of correlated quantum materials. He has investigated on electron-phonon coupling and pseudospin-lattice coupling, laser-induced electron coherence using SSPM, high pressure ultrafast dynamics, coherent phonon, squeezed magnon states, all-optical switching, photo-thermal-acoustic effect, etc

Training packages

Hefei-NAMD



Hefei-NAMD is an ab initio nonadiabatic molecular dynamics program to investigate the ultrafast excited carrier dynamics in real and momentum space, energy and time scale.
The source code can be download at:
https://github.com/QijingZheng/Hefei-NAMD .
For more information, please contact Dr. Qijing Zheng (zqj@ustc.edu.cn) or Prof. Jin Zhao (zhaojin@ustc.edu.cn)

TDAP

The Time-Dependent Ab-initio Package, or in its acronym 'TDAP', is aimed at carrying out real-time (rt) time-dependent density functional theory (TDDFT) calculations in efficient atomic bases. Such calculations allow first principles treatment of both electron and ion dynamics with non-adiabatic effects fully taken in account, by solving many-electron time-dependent Schrödinger equation. It enables large-scale first principles simulations of quantum dynamics in finite and extended systems including atoms, clusters, molecules, nanoparticles, solids, defects, interfaces, and two-dimensional materials, significantly reducing the heavy computational cost of typical rt-TDDFT simulations.
The academic licence can be obtained from:
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