复旦大学物理系物质科学报告

Introduction to first-principles simulation package

ABACUS

Physics Department Colloquium

Prof. He Lixin

Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei, 230026, China

Synergetic Innovation Center of Quantum Information and Quantum Physics,University of Science and Technology of China, Hefei, 230026, China

With the rapid development of supercomputers and the advances of numerical algorithms, nowadays it is possible to study the electronic, structural and dynamical properties of complicated physical systems containing thousands of atoms using density functional theory (DFT). The numerical atomic orbitals are ideal basis sets for large-scale DFT calculations in terms of their small base size and localized characteristic, and can be mostly easily combined with linear scaling methods. In this talk, we introduce a first-principles simulation package “Atomic-orbital Based Ab-initio Computation at UStc (ABACUS)”, developed at the Key laboratory of quantum information, University of science and technology of China, which provides a useful tool to study the electronic, structural and molecular dynamic properties of systems containing up to 1000 atoms. We show

a few examples of our recent first-principles simulations based on ABACUS.

个人简历：

何力新教授1994年毕业于中国科技大学物理系，并于1997年获中国科技大学硕士学位。 1998 - 2003 年在美国 Rutgers 物理系师从 David Vanderbilt 教授学习第一性原理的计算方法，并获博士学位。2003.9-2006.1 在美国国家再生能源实验室 Dr. Alex Zunger 领导的固体理论小组从事半导体量子点的理论研究工作。2006 年 1 月作为国外杰出人才（百人计划)引进至中国科技大学中科院量子信息重点实验室工作。 2010 年获基金委杰出青年科学基金。2012 年当选 IOP fellow （UK）。曾任科技部量子调控“量子通信网络和量子仿真关键器件的物理实现”(2011-2015) 首席科学家。

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Location：Physics Building, Room 221B

(Cookies and coffee are served from 1:45 pm)