Lectures on first-principles methods
Tsinghua University
Department of Physics

Time: 2019-05-19 8:30-12:30

Location: lecture Hall C302

Organized by Yong Xu, Department of physics, Tsinghua University

First-principles approaches to electronic band structure of materials

Hong Jiang(蒋鸿)

College of Chemistry, Peking University

北京大学化学与分子工程学院副教授、研究员。主要研究领域包括：1）基于格林函数的第一性原理多体理论方法发展；2）基于密度泛函理论框架的强关联体系的第一性原理方法；3）光电能量材料转化、分子磁性、过渡金属及其氧化物表面和多相催化的理论研究。

Abstract

In this work I will present our recent efforts to developing numer ically accurate and efficient first-principles based theoretical appro aches to electronic band structure of materials including numerica lly accurate GW approach in the linearized augmented planewaves (LAPW) framework, the perturbative (one-shot) modified Becke-Johnson potential method as a quick and pragmatic approach to el ectronic band structure of complex materials, and a non-empirical doubly screened hybrid functional approach that can treat both nar row-gap and wide-gap insulating systems accurately .

Van der Waals Interactions in Density Functional Theory and Their Contributions to the Design of novel Electronic Devices

Wei Liu(刘伟)

Nanjing University of Science and Technology

南京理工大学材料科学与工程学院教授，博士生导师，国家优秀青年科学基金获得者。主要研究领域包括：基于金属表面的、结构稳定的信息存储；金属及合金表面在催化反应中的作用机制；金属-有机复合界面热力学表征及动力学研究。

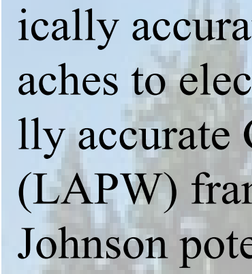
Abstract

In this talk I will first introduce the home-made DFT+vdWsurf met hod that accurately accounts for the collective electronic response effe cts enables reliable modeling of structure and stability for a broad clas s of organic molecules adsorbed on metal surfaces. Using the DFT+vd Wsurf method, I will further introduce some of our very recent findin gs in the design of functional (nanoscale) electronic devices. Special a ttentions will be paid on the push-button molecular switches, and Sch ottky diodes with tunable barrier heights.

Basics and State of the Art of Quantum-Chemistry Methods for Molecules, Clusters, and Materials

Igor Ying Zhang(张颖)

Department of Chemistry, Fudan University



复旦大学化学系研究员，青年千人，博士生导师。主要研究方向包括：1）高等密度泛函方法开发；2）偶合簇波函数方法开发；3）电子结构计算程序高性能并行设计；4）分子与固体测试集构建与分析；5）机器深度学习在电子结构方法开发中的应用。

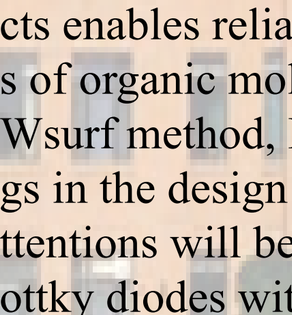
Abstract

The workhorse method of computational materials science is unden iably density functional theory (DFT) in the framework of approximat e exchange and correlation energy functionals. However, the need for highly accurate predictions of ground and excited state properties in m aterials science motivates the further development and exploration of alternative as well as complementary techniques. Among these alterna tive approaches, quantum chemical wave function based theories hold the promise to fill a gap in the toolbox of computational materials scie ntists. In this tutorial-style talk, I will introduce the basic concepts of quantum chemical methods and the recent advance in the field toward s the lower-scaling and massive-parallel implementation of quantum-chemistry methods for molecules, clusters, and materials.

Basics and Recent Progress of Random Phase Approximation for Electronic Ground-State Energy Calculations

Xinguo Ren(任新国)

CAS Key Laboratory of Quantum Information, University of Science and Technology of China



中国科学技术大学研究员，博士生导师。主要研究领域包括：密度泛函理论，特别是无规相近似及相关的先进交换关联泛函方法；格林函数理论，特别是基于GW近似的激发态计算方法；以及大型第一性原理计算软件的开发。

Abstract

The concept of random phase approximation (RPA) has a profound i mpact on both electronic structure theories and nuclear physics. A note worthy recent development of RPA is that it has been formulated and applied as a first-principles approach to calculate the electronic correla tion energy for molecules and materials. In this lecture, I will discuss t he basic concept of RPA and its typical applications in computational c hemistry and materials science. Recent and on-going developments, eit her on reducing the computational cost or adding corrections beyond R PA to further improve the accuracy, will also be briefly mentioned.