SEMINAR SERIES

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北京大学工学院材料科学与工程科学系

Nanostructure surface passivation and ligand induced surface morphology changes

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报告简介：

In this talk, I will present our recent work in studying surface ligand passivation, and the possible surface morphology changes due to ligand passivation. The first system is PbS quantum dot. We have studied the atomistic structure of surface PbS, and showing how ab initio calculation can be used to reveal the surface atomic structure, and the possible surface defect states of such systems. Another problem is surface passivation of metallic Pt nanocrystal. The ab initio calculation explain the mechanism of nanocrystal growth. It turns out that the growth is determined by kinetic process, instead of surface energy. The third example is CO coverage of Pt and Cu surface. It is found that such molecule coverage will induce morphology changes, thus will have major influence to their catalytic properties. Lastly, I will show how GPU calculations can be used to accelerate all the above calculations.

报告人：

Senior Staff Scientist, Lawrence Berkeley National Laboratory, Berkeley, CA, U.S. Dr. Wang has 25 years of experience in large scale electronic structure calculations. He has worked in O(N) electronic structure calculations in early 1990s. Worked with Alex Zunger, he invented the folded spectrum method which pushed the limit of nonselfconsistent electronic structure calculations from 100 atoms to thousands of atoms. He developed a linear combination of bulk bands (LCBB) method for semiconductor heterostructrure electronic structure calculations, which allows the calculation of million atom devices. He developed generalized moments method which calculates the density of state and optical absorption spectra of a given system without explicit calculation of its eigenstates. He also developed a popular parallel total energy plane wave pseudopotential program (PEtot). He invented a charge patching method, which enables the ab initio accuracy thousand atom calculations for nanosystems. He has developed a linear scaling three dimensional fragment method (LS3DF), which can be used to selfconsistently calculate systems with tens of thousands of atoms. Recently, he developed a new algorithm for real-time time-dependent DFT calculations which accelerates the traditional algorithms by hundreds of times.

主持人：孙强 教授

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地　点：工学院 1 号楼 210 会议室

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