Abstract of Presentation

Presentation Title:

Quantum simulations on nano-structured materials

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Abstract :

Nanoscience and nanotechnology have attracted enormous attention in recent years. At the nanometer length scale, matter behaves in a complex way and exhibits exotic properties, which are different from the behaviors of large-scale bulk systems. Besides, the behaviors of the nanoscale matter are in general difficult to measure by experiments. Based on the tremendous growth in computer power together with the development in simulation techniques such as optimized algorithms and computer codes, we are now able to predict the properties of matter theoretically from the fundamental laws of quantum mechanics, without any input from experiments. Thus, quantum simulations such as first-principles electronic structure calculations are expected to be powerful tools to investigate matter at the nanoscale and explore its potential applications for new devices.

In this talk, our recent activities of the development of first-principles simulation techniques and their applications for nano-structured materials are presented. The studies on the adsorption geometries and the diffusion pathways of atoms on semiconductor surfaces are presented in terms of energetics, which are crucial for the fabrication and control of nanostructures at the atomic level. We also show the results on the surface dynamics including the effect of energy dissipation, which are obtained by using a large-scale quantum-mechanical simulation technique, that is, a quantum-classical hybrid method. Molecular electronics has been rapidly emerging as a promising field of substantial technological interest. The investigations on exotic properties which small molecules exhibit are presented, including the studies on electrical transport through molecular wire junctions as well as on the femtosecond dynamics of photoexcited molecules. Finally, the linear scaling DFT calculation technique and its applications to nano-systems and bio-systems are also mentioned.