Final Technical Report

The Period of Performance, 7.15.11 to 5.31.17
The grant title: “Quantum Mechanical Simulations of Complex Nanostructures for Photovoltaic Applications”.
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The PI’s name: Dr. Zhigang Wu

Summary for the Period of Performance

In this project the PI investigated a chosen set of complex nanostructures that have great potential for opening new routes in designing materials with improved transport, electronic, and optical properties for PV and other optoelectronic usages. We focused on hybrid interfaces between materials with distinct electronic and optical properties, such as organic molecules (conjugated polymers, e.g. P3HT) and inorganic semiconducting materials (Si and ZnO). Complicated interface structures, including interface bonding configurations, compositional and geometrical blending patterns, interfacial defects, and various sizes and shapes of inorganic nanomaterials, was considered for the purpose of understanding the working mechanisms of present organic/nano PV systems and designing optimum interface structures for fast charge separation and injection, efficient energy transfer and transport. We also studied some complex-structured semiconducting nanomaterials, such as graphene nanomeshes (GNMs) and twisted/bent silicon nanowires, which could be tuned to obtain best or novel properties for optoelectronic applications and/or overcome certain difficulties. In order to carry out *ab initio* calculations for electronic, optical and transport properties of these complicated systems with very large unit cells, the PI tried to address the excited-state problem within the DFT framework to obtain quasiparticle energies from both Kohn-Sham (KS) eigenvalues and orbitals; and the electron-hole binding energy was considered to be computed based on the screened Coulomb interaction of corresponding DFT orbitals. The accuracy of these approaches was examined against many-body methods of GW/BSE and quantum Monte Carlo (QMC). The PI also worked on examining the accuracy and efficiency of the GW/BSE method and the hybrid functionals in electronic excitation computations. For ground-state properties, we compared DFT, quantum chemistry methods and QMC for nanostructures and small liquid clusters.

Publications Supported by This Fund

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