Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Quantum Monte Carlo Characterization of Excited States and Energy-Level Alignment of Oligomer/Quantum-Dot Interfaces[1]
JONATHAN DUBOIS, DONGHWA LEE, Lawrence Livermore National Laboratory, YOSUKE KANAI, The University of North Carolina, Chapel Hill — Charge separation of excitons in materials is one of the most important physical processes to utilize the solar energy in diverse devices including solar cells and photo-catalysts. Heterogeneous interfaces with the so-called type-II character are often employed to infer the interfacial charge transfer in this context. As a simple criterion for designing such an interface, the energy alignment of the quasi-particle states together with the exciton binding energy of electron-donating materials is often discussed in the literature. However, an accurate description of the effect of exciton binding at the interface has not been investigated extensively. Although density functional theory (DFT) is a powerful method to investigate various electronic properties of materials, incomplete description of many-body interactions can lead to an incorrect interpretation of the energy level alignment. While Many-Body Perturbation Theory and Quantum Monte Carlo are promising in this context, much more work is necessary to assess how well these methods perform in practice. In this talk, we will discuss our preliminary results using diffusion Quantum Monte Carlo to calculate the excited states and energy-level alignment at an Oligomer/Quantum-Dot interface – a system that is often discussed in context of solar energy conversion.

[1]This work is Prepared by LLNL under Contract DE-AC52-07NA27344.

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Date submitted: 20 Nov 2012 Electronic form version 1.4