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Quantum Monte Carlo Characterization of Excited States and Energy-Level Alignment at Oligomer/Quantum-Dot Interfaces YOSUKE KANAI, The University of North Carolina, Chapel Hill / Lawrence Livermore National Laboratory, JONATHAN L. DUBOIS, DONGHWA LEE, Lawrence Livermore National Laboratory — Charge separation of excitons in materials is one of the most important physical processes that need to take place in excitonic solar cells and in photocatalytic devices. Heterogeneous interfaces with the so-called type-II character are often employed for inducing the exciton dissociation through interfacial charge transfer. As the simplest criterion for designing such an interface, the energy alignment of the quasi-particle states is often discussed in literature, together with the exciton binding energy of electron-donating materials. Therefore, accurate characterization of the interfacial energy-level alignment and the exciton binding energy using first principles calculations is important for making systematic progresses in designing better materials for solar energy conversion. However, Density Functional Theory calculations need to be employed with caution in this context. First principles calculations such as Many-Body Perturbation Theory and Quantum Monte Carlo are promising alternatives for accurate characterization, but much more work is needed in this area to assess how well these methods perform in practice. In this talk, we will discuss our preliminary results using diffusion Quantum Monte Carlo on calculating the excited states and energy-level alignment of popular Oligomer/Quantum-Dot interfaces.

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