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First-principles studies of interfacial charge separation in nano-materials photovoltaic heterojunction[1]

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Charge separation is a crucial process that must be understood in order to make substantial improvements in nano-materials based PV cells. In our work, first principles quantum mechanical calculations are employed to shed light on this process for some important nano-material heterojunctions. I will first present our work on the interfacial charge separation in Fullerene/P3HT and CNT/P3HT heterojunctions. Our findings indicate that in the fullerene system a two-step process is operative, involving an adiabatic electron transfer and an exciton dissociation via quasi-degenerate states localized on the fullerene. For the nanotubes, on the other hand, while such a two-step process is not necessary for efficient charge separation, the presence of metallic nanotubes lead to undesirable charge traps. Secondly, I will discuss how we are addressing the difficulty in employing standard DFT approaches for investigating inorganic-organic PV interfaces, which are composed of two distinct materials with very different electronic environments. I will discuss a QMC scheme for obtaining many-body corrections to the Kohn-Sham level alignments and its application to a CdSe/Oligothiophene hybrid PV interface, with the aim of tailoring its behavior by controlling the conjugation length.

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