Electronic Structure of Dye-Sensitized TiO_2 Clusters from G_0W_0

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The development of new types of solar cells is driven by the need for clean and sustainable energy. In this respect dye sensitized solar cells (DSC) are considered as a promising route for departing from the traditional solid state cells. The physical insight provided by computational modeling may help develop improved DSCs. To this end it is important to obtain an accurate description of the electronic structure, including the fundamental gaps and level alignment at the dye-TiO_2 interface. This requires a treatment beyond ground-state density functional theory (DFT). In this talk I will present a many-body perturbation theory study, within the G_0W_0 approximation, of TiO_2 clusters, dye molecules, and dye-sensitized TiO_2 clusters. G_0W_0 calculations, based on a hybrid functional, are in excellent agreement with photoemission spectroscopy (PES) experiments. For TiO_2 clusters, this enables the identification of the isomers observed in PES as those with the highest vertical electron affinity [1]. For transition metal phthalocyanine dyes, unlike DFT, G_0W_0 calculations correctly predict the energies of orbitals associated with the metal d-states [2]. For dye-sensitized TiO_2 clusters, G_0W_0 calculations provide more reliable predictions than DFT for the fundamental gaps and the level alignment at the dye-TiO_2 interface [3].

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