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Size Effects in Dye-Sensitized TiO_2 Clusters NOA MAROM, Physics and Engineering Physics, Tulane University, New Orleans, LA, THOMAS KÖRZDÖRFER, Computational Chemistry, University of Potsdam, Potsdam, Germany, XINGUO REN, Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei, China, ALEXANDRE TKATCHENKO, Fritz Haber Institute of the Max Planck Society, Berlin, Germany, JAMES CHELIKOWSKY, Institute of Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX — The development of solar cells is driven by the need for clean and sustainable energy. Organic and dye sensitized cells are considered as promising technologies, particularly for large area, low cost applications. However, the efficiency of such cells is still far from the theoretical limit. *Ab initio* simulations may be used for computer-aided design of new materials and nano-structures for more efficient solar cells. It is essential to obtain an accurate description of the electronic structure, including the fundamental gaps and energy level alignment at the interfaces in the device active region. This requires going beyond ground-state DFT to the GW approximation. A recently developed GW method [PRB 86, 041110R (2012)] is applied to dye-sensitized TiO_2 clusters [PRB 84, 245115 (2011)]. The effect of cluster size on the energy level alignment at the dye-TiO_2 interface is discussed. With the increase in the TiO_2 cluster size its gap narrows. The gap of the molecule attached to the cluster subsequently narrows due to screening. As a result, the energy level alignment at the interface changes in an unexpected way [Marom, Körzdörfer, Ren, Tkatchenko, Chelikowsky, *to be published*].

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