

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional SIVAN REFAELY-ABRAMSON, Weizmann Institute of Science, Israel, ROI BAER, Hebrew University, Jerusalem, Israel, LEEOR KRONIK, Weizmann Institute of Science, Israel — The fundamental and optical gaps of relevant molecular systems are of primary importance for organic-based photovoltaics. Unfortunately, whereas optical gaps are accessible with time-dependent density functional theory (DFT), the highest -occupied - lowest-unoccupied eigenvalue gaps resulting from DFT calculations with semi-local or hybrid functionals routinely and severely underestimate the fundamental gaps of gas-phase organic molecules. Here, we show that a range-separated hybrid functional, optimally tuned so as to obey Koopmans' theorem, provides fundamental gaps that are very close to benchmark results obtained from many-body perturbation theory in the GW approximation. We then show that using this functional does not compromise the possibility of obtaining reliable optical gaps from time-dependent DFT. We therefore suggest optimally-tuned range-separated hybrid functionals as a practical and accurate tool for DFT-based predictions of photovoltaically relevant and other molecular systems. For more details, see S. Refaely-Abramson, R. Baer, L. Kronik, Phys. Rev. B 84, 075144 (2011).

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Date submitted: 05 Oct 2011

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