Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A non-empirical, parameter-free, hybrid functional for accurate calculations of optoelectronic properties of finite systems[1] NICHOLAS BRAWAND, Institute for Molecular Engineering, University of Chicago, MÁRTON VÖRÖS, Materials Science Division, Argonne National Laboratory and Institute for Molecular Engineering, University of Chicago, MARCO GOVONI, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — The accurate prediction of optoelectronic properties of molecules and solids is a persisting challenge for current density functional theory (DFT) based methods. We propose a hybrid functional where the mixing fraction of exact and local exchange is determined by a non-empirical, system dependent function. This functional yields ionization potentials, fundamental and optical gaps of many, diverse systems in excellent agreement with experiments, including organic and inorganic molecules and nanocrystals. We further demonstrate that the newly defined hybrid functional gives the correct alignment between the energy level of the exemplary TTF-TCNQ donor-acceptor system.

[1]DOE-BES: DE-FG02-06ER46262

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Date submitted: 11 Nov 2015 Electronic form version 1.4