Dielectric-dependent Density Functionals for Accurate Electronic Structure Calculations of Molecules and Solids

JONATHAN SKONE, Institute for Molecular Engineering, University of Chicago, MARCO GOVONI, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago Argonne National Laboratory — Dielectric-dependent hybrid [DDH] functionals [1] have recently been shown to yield highly accurate energy gaps and dielectric constants for a wide variety of solids, at a computational cost considerably less than standard GW calculations. The fraction of exact exchange included in the definition of DDH functionals depends (self-consistently) on the dielectric constant of the material. In the present talk we introduce a range-separated (RS) version of DDH functionals [2] where short and long-range components are matched using material dependent, non-empirical parameters. Comparing with state of the art GW [3] calculations and experiment, we show that such RS hybrids yield accurate electronic properties of both molecules and solids, including energy gaps, photoelectron spectra and absolute ionization potentials. [1] See, e.g. Skone et. al. PRB 89 195112 (2014) [2] Skone et. al. PRB (to be submitted) [3] Govoni and Galli JCTC 11 2680 (2015)

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