Abstract Submitted
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Dielectric-dependent Density Functionals for Accurate Electronic Structure Calculations of Molecules and Solids[1] 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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Jonathan Skone
University of Chicago

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