

Abstract Submitted
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Using Dielectric Properties to Design Nonempirical Hybrid Functionals for Accurate Electronic Structure¹ JONATHAN SKONE, Institute for Molecular Engineering, The University of Chicago; Materials Science Division, Argonne National Laboratory, MARCO GOVONI, Institute for Molecular Engineering, The University of Chicago, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago; Materials Science Division, Argonne National Laboratory — Building upon a recently proposed self-consistent hybrid (sc-hybrid) functional [1], where the optimal dielectric screening is included self-consistently, we propose an improved form by incorporating range-separation of the exchange part. We discuss the choice of the non-empirical parameters defining range separation, and we present results for condensed media including semiconductors, amorphous insulators, and molecular crystals. We find that the range-separated sc-hybrid functional further improves upon the electronic gaps obtained with full-range sc-hybrids, thus providing an accurate functional for high throughput band gap engineering.

[1] Skone, Govoni, and Galli PRB 89 195112 (2014).

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