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Approximations in local hybrid density functionals BENJAMIN JANESKO, Rice University, GUSTAVO SCUSERIA, Rice Unveristy — Hybrid density functionals incorporating a fraction of exact (Hartree-Fock-type) electronic exchange have become one of the dominant approximations for modeling the electronic structure of large molecules and solids. Generalization to a position dependent admixture of exact exchange provides a route to improved accuracy. However, such local hybrid functionals generally have a significant computational expense. We present work towards approximate density functionals that incorporate some of the desirable properties of local hybrids, without requiring explicit evaluation of exact exchange. These results show promise for extending the benefits of hybrid functionals to larger systems.

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