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Self-optimizing Kohn-Sham hybrid functional ISAAC TAMBLYN, Molecular Foundry, LBNL, ROI BAER, Hebrew University, Jerusalem, LEEOR KRONIK, Weizmann Institute of Science, Israel, JEFFREY NEATON, Molecular Foundry, LBNL — Recent work using range-separated hybrid functionals has confirmed the importance of including long-range exchange in treatments of phenomena such as charge transfer reactions. Using a self-optimizing [1,2] form of the BNL [3] functional, we present results for structural, electronic, and thermochemical properties of a large set of molecules (including the G2 and G3 test sets). The success of this approach, as well as its ability to describe reaction barriers, will be discussed.

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[2] T. Stein, H. Eisenberg, L. Kronik, and R. Baer, "Fundamental gaps of finite systems from the eigenvalues of a generalized Kohn-Sham method", Phys. Rev. Lett., in press.
[3] E. Livshits and R. Baer, PCCP, 9, 2932 , 2007

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