THINKING BIG AND SMALL: PREDICTING MOLECULAR AND EXTENDED SYSTEM PROPERTIES USING THE QTP FAMILY OF FUNCTIONALS

Zachary W. Windom*†, Ajith Perera*†, Rodney Bartlett*†

*Department of Chemistry, University of Florida, Gainesville, FL USA
†Quantum Theory Project, University of Florida, Gainesville, FL USA

Due to its favorable scaling and relatively high accuracy, Kohn-Sham Density Functional Theory (DFT) has transitioned into a dominating workhorse of quantum chemistry that is routinely applied in the study of chemical structure and reactivity while encompassing a variety of fields ranging from the vapor and condensed phases, as well as the solid state. In spite of this the exchange-correlation potential of conventional DFT face significant hurdles, for example, in minimizing the self-interaction error, obtaining the qualitatively correct one particle spectrum, and rectifying the delocalization error of many electron systems. However, by reparamaterizing existing functionals to satisfy the DFT analog of Koopman's theorem, the Quantum Theory Project (QTP) line of density functionals has proven successful in mitigating these issues in addition to correctly describing a variety of phenomena ranging from vertical excitation and charge-transfer energies to reaction barrier heights. Here, we present a further examination of the capabilities for the range-separated QTP-00, QTP-01, and QTP-02 functionals in describing the band structure of select materials as well as the isotropic hyperfine coupling of 23 radical molecules. Preliminary results suggest that the QTP family of functionals predict the experimental band gap while also offering competitive results for Fermi contact, as compared to a myriad of standard DFT functionals and CCSD(T) results. To convey the universality of the IP condition, we show that by reparameterizing the PBE0 functional based only on the IP and EA of the water and hydroxyl molecules, the resulting global hybrid functional (QTP-PBE0) exhibits an improvement in predicting extended systems' band gap.