Alchemical perturbation density functional theory

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We introduce an orbital free electron density functional approximation based on alchemical perturbation theory. Given convergent perturbations of a suitable reference system, the accuracy of popular self-consistent Kohn-Sham density functional estimates of properties of new molecules can be systematically surpassed—at negligible cost. The associated energy functional is an approximation to the integrated energy derivative, requiring only perturbed reference electron densities: No self-consistent field equations are necessary to estimate energies and electron densities. Electronic ground state properties considered include covalent bonding potentials, atomic forces, as well as dipole and quadropole moments.
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