Progress at the interface of wave function and density functional theories.

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The Kohn Sham (KS) potential of Density Functional Theory emerges as the minimizing effective potential in a Rayleigh Ritz energy minimization that does not involve fixing the unknown single electron density. In particular, we take that the exact ground state Psi of the interacting N electron system is known and we consider the class of effective non-interacting Hamiltonians, Hv = T + V, characterized by the local multiplicative potential V. The search for the effective local multiplicative potential V, such that the expectation value of Hv in terms of Psi is closest to the actual ground state energy of Hv, yields the KS potential as the optimal potential.
Based on the new Rayleigh Ritz minimization above, and using finite order perturbation theory to write Psi formally, one may construct ab initio expressions for the energy difference whose minimization yields the KS potential. In this way, we generate variationally stable series expansions for the KS potential.