Multiconfiguration Nonclassical-Energy Density Functional Theory

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ABSTRACT. Multiconfiguration nonclassical-energy functional theory (MC-NEFT) [1] is a low-cost and high-accuracy electronic structure method to recover dynamic correlation in inherently multiconfigurational species. In MC-NEFT, one starts with a multiconfigurational wave function, usually a multiconfiguration self-consistent-field (MCSCF) wave function, such as a complete active space self-consistent field (CASSCF) wave function, that recovers the static correlation and typically a small portion of the dynamic correlation. Then, a nonclassical energy functional is used to calculate the energy from some properties of the multiconfigurational wave function. The use of a nonclassical energy functional greatly reduces the computational cost compared to traditional post-CASSCF methods such as multireference perturbation theory or multireference configuration interaction while having comparable or better accuracy in terms of bond dissociation energy, reaction barrier height, and excitation energies. The talk will cover MC pair-density FT (MC-PDFT) [2}, hybrid MC-PDFT [3], hybrid meta PDFT [4}, data -driven PDFT [5}, hybrid density coherence FT [6], and linearized PDFT [7] including recent developments.

References

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