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All-Electron and Pseudopotential Orbital-Free Density Functional Calculations[1] VALENTIN KARASIEV, T. SJOSTROM, S.B. TRICKEY, Physics, QTP, Univ. Florida — Generalized gradient approximation (GGA) and modified-conjoint GGA kinetic energy functionals, proposed recently, have been implemented in an all-electron diatomic molecule code and in a periodic boundary condition code which uses local pseudopotentials. Self-consistent OF-DFT calculations confirm earlier non-self-consistent results. The GGA KE functionals give qualitatively incorrect total energy surfaces in the attractive region (isolated molecule) and the equilibrium crystalline cell volume is strongly expanded. In contrast, the mcGGA functional predicts a qualitatively correct energy surface for isolated systems, and the equilibrium geometry for pseudopotential calculations is in agreement with the Kohn-Sham results. We show the closeness in behavior between GGA-based functionals and simpler approximations defined by mixing of the Thomas-Fermi and the von Weizsäcker KE functionals. Effects of the pseudopotential in OF-DFT calculations also are discussed.

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