Semiclassical atom theory applied to solid-state physics

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Using the semiclassical neutral atom theory [1,2], we extend to fourth order the modified gradient expansion of the exchange energy of density functional theory [3]. This expansion can be applied both to large atoms and solid-state problems, being significantly better than the conventional fourth-order gradient expansion of the exchange energy [3].

We show that this gradient expansion can be employed to construct a simple and nonempirical generalized gradient approximation (GGA) exchange-correlation functional, named the semiclassical GGA at fourth order (SG4). The SG4 GGA is competitive with state-of-the-art GGAs for solids, being one of the best functional for equilibrium lattice constants, bulk moduli, cohesive energies, surface energies and monovacancy formation energies of strongly-bounded solids [3]. Moreover, the SG4 GGA is also reasonably accurate for large atoms and ordinary chemistry [3].

When SG4 GGA is combined with the van der Waals non-local correction, the resulting functional preserves the high accuracy of SG4 GGA for strongly-bounded solids, and becomes very accurate for layered materials, and van der Waals solids [4].

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