Non-empirical semilocal functionals for improved performance in quantum chemistry and materials science

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The research in the field of semilocal exchange-correlation (XC) functionals is continuously asking for improved accuracy, broader applicability, and reduced empiricism. In this contribution we present our recent developments in this direction, by reporting on four *non-empirical* semilocal functionals: PBEint, zPBEint, APBE, Q2D-GGA.

The PBEint functional [1] was constructed to correctly reproduce both the slowly- and the rapidly-varying density regimes. Therefore, it performs well both for molecular and solid-state problems [2,3] and describes jellium surfaces energies without error cancellation between exchange and correlation [3]. It is especially suited to study complex problems where both density regimes coexist (e.g. hybrid interfaces, molecules on surfaces [1], metallic clusters [4]). The PBEint functional is implemented in the current version of FHI-AIMS.

The zPBEint functional [5], was designed as an extension of the PBEint functional to improve the description of spin-polarized systems, without modifying the accuracy for closed-shell cases. It significantly enhances the description of atomic and molecular open-shell systems thus improving the description of atomization and cohesive energies.

The APBE functional [6] was developed using the asymptotic expansion of the semiclassical atom. It provides very accurate results for atomic and molecular properties, and still performs well for solid-state systems. Moreover, the APBE functional is one of the most accurate semilocal approximations for the description of hydrogen bonds [2].

Finally, the Q2D-GGA functional [7] is a semilocal approximation for quasi-two-dimensional (Q2D) systems. It satisfies the nonuniform scaling in one dimension and is accurate in the whole (Q2D) regime as well as for bulk systems. The Q2D-GGA functional was shown to perform well for solid-state problems and in particular to be a valuable tool for the calculation of surface energies of many transition-metal surfaces.

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