Electron correlation via the adiabatic-connection dissipation-fluctuation theorem and temperature-dependent exact exchange

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Electronic structure methods using orbital-dependent exchange-correlation functionals within the Kohn-Sham (KS) formalism of density-functional theory are introduced. An approach to treat the KS exchange energy and potential exactly in the case of non-zero temperature is presented and applied to describe topological phase transitions in zinc-blende compounds [1,2]. The treatment of electron correlation based on the adiabatic-connection fluctuation-dissipation theorem is discussed [3,4] and a new class of correlation functionals, named sigma-functionals, is presented [5]. Technically, sigma-functionals are very similar to functionals within the well-known random phase approximation and have similar computational demands. The accuracy of sigma-functionals, however, is substantially higher than that of functionals within the random-phase approximation. Indeed, reaction and transition state energies of molecules from various established test sets as well as Van-der-Waals binding energies from sigma-functionals are as accurate as those from high level quantum quemistry methods [5] that are computationally much more demanding and therefore quite limitied in their range of application. Sigma-functionals therefore open up new areas of application for KS methods in chemistry, physics, and materials science.

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