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Advances in density−functional theory by orbital and state dependent functionals

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A new Kohn−Sham (KS) formalism, the symmetrized generalized adiabatic connection KS formalism, is introduced. It is applicable to ground as well as excited states and does not suffer from the symmetry problems of the standard KS approach. In all cases a totally symmetric, non−spin−polarized KS Hamiltonian operator arises. Complete electronic spectra, including multiplet splittings, Rydberg series, X−Ray and Auger data can be described. Results for the carbon atom and the carbonmonoxide molecule are presented.

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