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Optimized effective potential methods for molecules and solids

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The relation of the optimized effective potential (OEP) method to density-functional theory and in particular to Kohn-Sham (KS) methods is discussed. It is shown that OEP approaches only represent proper KS methods if the basis set for the one-particle functions and the basis set for the effective potential are well balanced. It is shown that exact exchange KS methods based on the OEP approach not only yield band structures that are improved compared to band structures resulting from conventional KS approaches but that exact exchange magnetization-current density-functional theory implemented via an OEP approach represents a framework for a unified treatment of magnetic effects, spin-orbit interactions, and magnetization currents.