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New ways of computing effective potentials for orbital-dependent functionals VIKTOR N. STAROVEROV, The University of Western Ontario — Orbital-dependent density functionals offer many advantages over local-density and gradient-corrected approximations, but also pose distinctive challenges to developers and users alike. In particular, evaluation of functional derivatives of orbital-dependent functionals is far from straightforward because of numerical difficulties and basis-set artifacts involved. In response to this challenge, we have developed a whole class of iterative methods for accurate and efficient calculation of Kohn-Sham potentials for various orbital-dependent functionals including exact exchange, hybrids, and meta-generalized gradient approximations. The presentation will overview these methods and demonstrate their dramatic advantage over existing approximations (KLI, LHF, etc.) in practical finite-basis-set calculations.

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