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**Iterative minimization by Kohn–Sham inversion and potential mixing** ROOPE ASTALA, MALCOLM STOTT, Department of Physics, Queen's University, Kingston, Ontario, Canada — Applications of Hohenberg–Kohn–Sham density functional theory to problems in materials physics are critically dependent on algorithms for iterating the Kohn–Sham equations to self-consistency. We present an approach for obtaining the self-consistent solution, which explores a connection between iterative minimization and Kohn–Sham inversion, *i.e.* finding a self-consistent potential for a given density. The central idea is to perform the Kohn–Sham inversion using a position-dependent Lagrange multiplier and to construct a new trial potential from the result. The method is variational, in contrast to commonly-used density mixing approaches, and has excellent convergence. We demonstrate the method using a real-space pseudopotential implementation with applications to small molecules.

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