Abstract Submitted
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Non-linear eigensolver-based alternative to traditional SCF methods[1] BRENDAN GAVIN, ERIC POLIZZI, Univeristy of Massachusetts, Amherst — The self-consistent iterative procedure in Density Functional Theory calculations is revisited using a new, highly efficient and robust algorithm for solving the non-linear eigenvector problem (i.e. H(X)X = EX;) of the Kohn-Sham equations. This new scheme is derived from a generalization of the FEAST eigenvalue algorithm, and provides a fundamental and practical numerical solution for addressing the non-linearity of the Hamiltonian with the occupied eigenvectors. In contrast to SCF techniques, the traditional outer iterations are replaced by subspace iterations that are intrinsic to the FEAST algorithm, while the non-linearity is handled at the level of a projected reduced system which is orders of magnitude smaller than the original one. Using a series of numerical examples, it will be shown that our approach can outperform the traditional SCF mixing techniques such as Pulay-DIIS by providing a high converge rate and by converging to the correct solution regardless of the choice of the initial guess. We also discuss a practical implementation of the technique that can be achieved effectively using the FEAST solver package.

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