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A Unified Software Interface to Solve or Circumvent the Kohn-Sham Eigenvalue Problem: ELSI VICTOR YU, WILLIAM HUHN, BJÖRN LANGE, VOLKER BLUM, MEMS Dept., Duke Univ., FABIANO CORSETTI, Dept. of Materials, Imperial College London, LIN LIN, Dept. of Mathematics, UC Berkeley, JIANFENG LU, Dept. of Mathematics, Duke Univ., ALVARO VAZQUEZ-MAYAGOITA, Argonne National Laboratory, CHAO YANG, Lawrence Berkeley National Laboratory — Solving or circumventing a generalized eigenvalue problem is often the bottleneck in large scale calculations based on Kohn-Sham density-functional theory (KS-DFT). This problem must be addressed by essentially all current electronic structure codes, based on similar matrix expressions, and by high-performance computation. We here present a unified software interface, ELSI, to simplify the access to existing strategies to address the KS eigenvalue problem. Supported algorithms include the massively parallel dense eigensolver ELPA ($O(N^3)$), the orbital minimization method in libOMM ($O(N^3)$ with a reduced prefactor), and the Pole EXpansion and Selected Inversion (PEXSI) approach with lower computational complexity (at most $O(N^2)$). The ELSI interface aims to simplify the implementation and optimal use of the different strategies, by a) optional automatic selection of the correct solver depending on the specific problem; b) reasonable default parameters for a chosen solver; and c) automatic conversion between input and internal working matrix formats. Benchmarks are shown for all-electron Hamilton and overlap matrices for system sizes up to several thousand atoms. This work is supported by the National Science Foundation under Grant Number 1450280.

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