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The pole expansion and selected inversion technique for solving Kohn-Sham density functional theory at large scale[1] LIN LIN, Lawrence Berkeley National Laboratory, MOHAN CHEN, WEINAN E, Princeton University, LIXIN HE, University of Science and Technology of China, JIANFENG LU, Duke University, CHAO YANG, Lawrence Berkeley National Laboratory, LEXING YING, University of Texas at Austin — The standard diagonalization based method for solving Kohn-Sham density functional theory (KSDFT) requires N eigenvectors for an O(N) * O(N) Kohn-Sham Hamiltonian matrix, with N being the number of electrons in the system. The computational cost for such procedure is expensive and scales as $O(N^3)$. We have developed a novel pole expansion plus selected inversion (PEXSI) method, in which KSDFT is solved by evaluating the selected elements of the inverse of a series of sparse symmetric matrices, and the overall algorithm scales at most $O(N^2)$ for all materials including metallic and insulating systems without any truncation. The PEXSI method can be used with orthogonal or nonorthogonal basis set, and the electron density, total energy, Helmholtz free energy and atomic force are calculated simultaneously and accurately without using the eigenvalues and eigenvectors. Combined with atomic orbital basis functions, the PEXSI method can be applied to study the electronic structure of boron nitride nanotube and carbon nanotube with more than 10,000 atoms on a single processor.

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