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A robust and monotonically convergent iterative algorithm for solving the Kohn-Sham equations in metallic systems[1] JEAN-LUC FATTEBERT, Lawrence Livermore National Laboratory — We propose a new iterative algorithm to efficiently calculate the electronic structure in Density Functional Theory calculations of metallic systems and warm dense matter with high electronic temperature. This parameter-free algorithm directly searches for a set of wave functions and a compatible single particle density that minimizes the Mermin finite temperature functional. It is particularly useful for simulating physical systems considered difficult to converge, such as large systems with variable occupancies and presenting charge sloshing. We demonstrate the effectiveness of the proposed algorithm and its implementation by applying it to challenging large scale problem in First-Principles Molecular Dynamics simulations.

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