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Periodic Density Functional Theory Solver using Multiresolution Analysis with MADNESS[1] ROBERT HARRISON, Oak Ridge National Laboratory, WILLIAM THORNTON, University of Tennessee — We describe the first implementation of the all-electron Kohn-Sham density functional periodic solver (DFT) using multi-wavelets and fast integral equations using MADNESS (multiresolution adaptive numerical environment for scientific simulation; http://code.google.com/p/m-a-d-n-e-s-s). The multiresolution nature of a multiwavelet basis allows for fast computation with guaranteed precision. By reformulating the Kohn-Sham eigenvalue equation into the Lippmann-Schwinger equation, we can avoid using the derivative operator which allows better control of overall precision for the all-electron problem. Other highlights include the development of periodic integral operators with low-rank separation, an adaptable model potential for nuclear potential, and an implementation for Hartree Fock exchange.

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