

Abstract Submitted
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Density Functional Theory using Multiresolution Analysis with MADNESS SCOTT THORNTON, ROBERT HARRISON, Joint Institute for Computational Sciences — 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 multi-wavelet 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 the nuclear potential, and an implementation for Hartree-Fock exchange.

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