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Exact Exchange calculations for periodic systems: a real space approach AMIR NATAN, NOA MAROM, ADI MAKMAL, LEEOR KRONIK, Weizmann Institute of Science, Israel, STEPHAN KUEMMEL, Bayreuth University, Germany — We present a real-space method for exact-exchange Kohn-Sham calculations of periodic systems. The method is based on self-consistent solutions of the optimized effective potential (OEP) equation on a three-dimensional non-orthogonal grid, using norm conserving pseudopotentials. These solutions can be either exact, using the S-iteration approach, or approximate, using the Krieger, Li, and Iafrate (KLI) approach. We demonstrate, using a variety of systems, the importance of singularity corrections and use of appropriate pseudopotentials.

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