Real-Space Screened-Exchange Method for Large Systems TITUS SANDU, MARK VAN SCHILFGAARDE, Chemical and Materials Engineering Department, Arizona State University, Tempe, AZ — A self-consistent screened exchange method in real-space has been developed for electronic structure calculations. Both static polarization function P0 and self-energy sigma are calculated in real space using Green’s function within TB-LMTO (tight-binding linear muffin-tin orbital) method. The method is fast and does not require orthogonal orbitals, enabling us to handle large systems. We compare the results for GaAs in zincblende structure, MnAs with NiAs-type structure, and Ga₃MnAs₄ in zincblende structure with those results obtained from GW approximation. Finally, the method is applied to diluted Ga(1-x)Mn(x)As.

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