Abstract Submitted
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MP2 calculations for solid state systems[1] MARTIJN MARSMAN, GEORG KRESSE, Faculty of Physics, University Vienna, and Center for Computational Materials Science — We present *ab initio* total energy calculations at the level of Hartree-Fock + 2nd-order Møller-Plesset perturbation theory (HF+MP2) for extended systems using periodic boundary conditions and a plane wave basis set. To characterize the accuracy of this level of theory, HF+MP2 lattice constants, bulk moduli, and atomizations energies for several archetypical semiconducting and insulating solid state systems are compared to those from density functional theory calculations and experiment. The HF+MP2 description of van der Waals interactions is illustrated for several noble gas solids. Important computational aspects of HF+MP2 calculations within the plane wave full potential projector-augmented-wave (PAW) formalism, most notably the basis set extrapolation of the MP2 correlation energy, are addressed as well.

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