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Hybrid functional description of the rhombohedrally distorted B1-structured MnO CESARE FRANCHINI, Institute of Physical Chemistry, Center for Computational Material Science, University of Vienna - Austria, ROBIN HIRSHL, GEORG KRESSE, Institut fuer Materialphysik, Center for Computational Material Science, University of Vienna - Austria, VERONIKA BAYER, RAIMUND PODLOUCKY, Institute of Physical Chemistry, Center for Computational Material Science, University of Vienna - Austria — We report a first principle calculation of the ground state properties of MnO within the plane wave based PBE0 hybrid density functional approach developed on the projector augmented wave scheme VASP (Vienna *ab initio* Simulation Package). The insulating, antiferromagnetically ordered and rhombohedrally distorted B1 structure is found to be the most stable phase, consistent with experiment. The gap (4.02 eV), magnetic moment (4.52 m_B), optimum lattice constant (4.40 A), rhombohedral distortion angle (0.88), density of states, and exchange integrals, are all in good agreement with experiment. Our findings confirm the picture which places MnO in the intermediate charge-transfer/Mott-Hubbard regime and suggest that the parameter-free PBE0 hybrid functional method, combining the full nonlocal exact exchange interaction with the PBE exchange-correlation functional well correct the deficiency of conventional DFT, thus providing a accurate description of this correlated material.

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