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All-electron Hybrid Functional Treatment of Oxides using the FLAPW Method MARKUS BETZINGER, MARTIN SCHLIPF, CHRISTOPH FRIEDRICH, MARJANA LEŽAIĆ, STEFAN BLÜGEL, Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — Hybrid functionals are a practical approximation for the exchange-correlation (xc) functional of density-functional theory. They combine a local or semi-local xc functional with nonlocal Hartree-Fock (HF) exchange and improve the band gap for semiconductors and insulators as well as the description of localized states. So far, most implementations for periodic systems employ a pseudopotential planewave approach. We present an efficient all-electron implementation in the context of the FLAPW methodology realized in the `FLEUR` (www.flapw.de) code. We report on the implementation of the PBE0 and HSE functionals where an auxiliary basis is constructed from products of LAPW basis functions and used to calculate the HF potential. The Coulomb matrix[1] then has a sparse form. Spatial and time-reversal symmetry is exploited in restricting the Brillouin zone sum in the nonlocal potential to an irreducible wedge. We give account on the efficiency of our concept and of the convergence of the self-consistency cycle. Finally we present results for a variety of oxides and compare those to results obtained with functionals based on the generalized gradient approximation. [1] *Comput. Phys. Comm.* **180**, 347 (2009)

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