Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

All-electron *GW* calculations for perovskite transition-metal oxides CHRISTOPH FRIEDRICH, ANDREAS GIERLICH, STEFAN BLÜGEL, Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany, ARNO SCHINDLMAYR, Department Physik, Universität Paderborn, 33095 Paderborn, Germany — The *GW* approximation for the electronic self-energy, which combines bare exchange with the dynamical screening of the many-electron system within the random-phase approximation, yields quasiparticle band structures in very good agreement with experiment. While most implementations today employ the pseudopotential approximation, our recently developed realization (http://www.flapw.de/spex) is based on the all-electron full-potential linearized-augmented-planewave (FLAPW) method, where core and valence electrons are treated on the same footing. Within this method a large variety of materials can be studied, including d- and f-electron systems, oxides and magnetic systems. In this work we present results for selected perovskite transition-metal oxides, such as $SrTiO_3$, $BaTiO_3$, $PbTiO_3$ and others, which are widely used in technical applications. Their band gaps are difficult to measure experimentally and have been under debate for a long time. Most ab-initio studies so far were based on density-functional theory and showed a strong underestimation of the band gap. Our all-electron *GW* calculations overcome this problem and yield band gaps very close to experiment.

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Date submitted: 08 Dec 2009 Electronic form version 1.4