Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Efficient all-electron *GW* calculations of complex semiconductors[1]
CHRISTOPH FRIEDRICH, Forschungszentrum Juelich, Germany, ARNO SCHINDLMAYR, Universitaet Paderborn, Germany, STEFAN BLÜGEL, Forschungszentrum Juelich, Germany — The *GW* approximation for the electronic self-energy yields quasiparticle band structures in very good agreement with experiment, but almost all implementations so far are based on the pseudopotential approach, which limits their range of applicability. We have developed an implementation (SPEX, http://www.flapw.de/spex/) within the all-electron full-potential linearized augmented-plane-wave (FLAPW) method. Within this method a large variety of materials can be treated, including d- and f-electron systems, oxides and magnetic systems. Our implementation employs a mixed product basis for the representation of wave-function products. A basis transformation to the eigenfunctions of the Coulomb potential allows a reduction of the basis-set size without compromising the accuracy, thus leading to a considerable speed-up in computation time. To demonstrate the efficiency of the implementation we present results for complex semiconductors.

[1]Financial support from the Deutsche Forschungsgemeinschaft through the Priority Programme 1145 is gratefully acknowledged.

Christoph Friedrich
Forschungszentrum Juelich

Date submitted: 21 Nov 2008 Electronic form version 1.4