Efficient all-electron implementation of the GW approximation within the full-potential linearised augmented-plane-wave method

Christoph Friedrich[1], **Arno Schindlmayr**[2], **G. Bihlmayer**[1], **and Stefan Blügel**[1]

[1] Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

[2] Department Physik, Universität Paderborn, 33095 Paderborn, 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 within the full-potential linearised augmented-plane-wave (FLAPW) method, which treats core and valence electrons on an equal footing. 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 basis-function products in the interstitial and muffin-tin regions. An expansion of the wave functions around the Γ point using $\mathbf{k}\cdot\mathbf{p}$ perturbation theory allows us to treat the divergence of the Coulomb interaction analytically leading to fast convergence with respect to the $\mathbf{k}$-point sampling. The anisotropy of the dielectric screening is fully taken into account. A basis transformation to the eigenfunctions of the Coulomb potential allows a reduction of the basis-set size without compromising the accuracy, which leads to a considerable speed-up in computation time. As a demonstration we show results for prototype semiconductors and insulators, perovskite transition-metal oxides, and ferromagnetic nickel. Financial support from the DFG through the Priority Programme 1145 is gratefully acknowledged.