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GW Calculations Starting from Generalized Kohn-Sham Schemes FRANK FUCHS, JÜRGEN FURTHÜLLER, FRIEDHELM BECHSTEDT, Friedrich-Schiller-University Jena, Germany, MAXIM SHISHKIN, GEORG KRESSE, CMS University Vienna, Austria — The GW approximation of Hedin is arguably the most successful approach for the calculation of quasi-particle (QP) energies. Its accuracy has been proven for a variety of systems. Usually, the QP eigenvalues are calculated in a perturbative approach, starting from solutions of the Kohn-Sham equations with an exchange-correlation (XC) potential in local density or generalized gradient approximation (LDA/GGA). However, this standard approach fails for a number of systems such as InN with shallow 'semi-core' electrons and a 'negative gap' in LDA/GGA. Here we present G_0W_0 calculations for Si, ZnO and InN which start from solutions of the generalized Kohn-Sham (gKS) equations for the screened exchange (sX), HSE03, PBE0 and HF model of exchange and correlation. The calculations are performed in the all-electron wavefunction framework of the PAW method. Starting from a gKS solution is found to yield a positive gap and d -band positions close to the experimental values for all the functionals investigated here. Furthermore, with exception of HF the resulting gaps are almost the same for all the gKS functionals chosen as starting point. The results are analysed with respect to the wave-function character and localization.

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