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Quasiparticle Corrections to the Electronic Properties of Point Defects[1] ARNO SCHINDLMAYR, Forschungszentrum Jülich and Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, MAGNUS HEDSTRÖM, PHILIPP EGGERT, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — We present a quantitative ab initio method for calculating defect states and charge-transition levels of point defects in semiconductors. It relies on a separation into lattice and electronic energy contributions, which are treated within density-functional theory and many-body perturbation theory, respectively. We use the *GW* approximation for the self-energy to determine the quasiparticle corrections to defect states in the band gap. As an example, we consider anion vacancies on the (110) surfaces of III-V semiconductors. The calculated charge-transition levels, in particular, show a clear improvement over the local-density approximation and are in close agreement with the available experimental data. As the surface is simulated by a slab within the supercell approximation, we place special emphasis on a convergence analysis of the quasiparticle properties in this approach. The dynamic polarization between the periodic images can be understood within a simple model, which also allows an a posteriori correction.

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