Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Constructing the GW self-energy of a point defect from the perfect crystal and the near neighborhood of the defect[1] DMITRY SKACHKOV, Case Western Reserve University, Cleveland, OH USA, MARK VAN SCHILFGAARDE, Kings College London, London, United Kingdom, WALTER LAMBRECHT, Case Western Reserve University — The full-potential linearized muffin-tin orbital method allows for a real space representation of the GW or quasiparticle self-consistent (QS)GW self-energy $\Sigma_{\mathrm{R,L;R'+T,L'}}$. This can be used to construct the self-energy matrix for a point defect system in a large supercell from that of the perfect crystal in the primitive cell and the self-energy of the defect site and its near neighborhood, obtained self-consistently in a smaller supercell. At the interface between both regions we can average the two types of $\Sigma_{\mathrm{R,L;R'+T,L'}}$ matrix blocks. The result relies on the limited range of the self-energy matrix in real space. It means that we can calculate the quasiparticle energy levels of the defect system at essentially the cost of a DFT calculation and a few QSGW calculations for relatively small systems. The approach presently focuses on quasiparticle energy levels of band structures of the defect system rather than total energies. We will present test results for $\mathrm{As_{Ga}}$ in GaAs, $\mathrm{Zn_{Ge}}$ in $\mathrm{ZnGeN_2}$, $\mathrm{N_O}$, $\mathrm{V_O}$, $\mathrm{V_{Zn}}$, and $\mathrm{N_O{-}V_{Zn}}$ in ZnO.

[1]Supported by the US-DOE-BES under Grant No. DE-SC0008933.

Dmitry Skachkov
Case Western Reserve University, Cleveland, OH USA

Date submitted: 20 Nov 2016 Electronic form version 1.4