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Self-consistent band-structure calculations at GW quality and DFT expense[1] STEPHAN LANY, P. GRAF, M. D'AVEZAC, A. ZUNGER, Natl. Renewable Energy Lab., CO — GW provides rather accurate quasi particle energies where approximate DFT methods tend to fail, yet are too computer intensive for complex inorganic materials (large systems or dense Brillouin zone sampling) that are currently of interest, e.g. for energy conversion. We explore the possibility that the trends of the GW quasi-particle energy corrections due to the non-local and energy dependent self-energy Σ(r,r',E) can be captured by atomic potentials that do not significantly increase the computational effort of a standard DFT calculation. We proceed in 4 steps: (i) Perform GW reference calculations for II-VI and III-V semiconductors (ii) Define atomic potentials that are added to the DFT Hamiltonian. Here we extend the concept of the non-local external potentials (NLEP) of Ref. [1], now allowing for two parameters per atom type and angular momentum. (iii) Fit the NLEP parameters to the GW test set. (iv) Finally, we test transferability by applying the potentials to the III_2-VI_3 and II_3-V_2 compounds that were not included in the fitting set.

[1] S. Lany, H. Raebiger, A. Zunger, Phys. Rev. B 77, 241201(R) (2008).

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