

Layer-projected scissors operator to simulate GW band structures of van der Waals heterostructures

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We introduce an efficient method to simulate the GW band structures of van der Waals heterostructures. GW calculations are notoriously computationally demanding, and large heterostructure supercells (due to lattice mismatch) are unreachable by standard GW calculations. Our method simulates the GW quasiparticle band structure of these supercells utilizing the layer projected self-consistent scissors operator (LAPS), requiring only GW calculations of unit cells of the individual layers as an input. In addition to accounting for band edge energies with the novel layer projected scissors operator, we also add the image charge correction utilizing the quantum electrostatic heterostructure (QEH) model [1-3]. In addition, corrections for excess strain due to utilization of finite heterostructure supercells are also included. The method is implemented to the GPAW open source electronic structure software [4,5].

References

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Figures

