

Faster GW Calculations in Larger Model Structures Using Ultralocalized Nonorthogonal Wannier Functions

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We introduce a novel approach for performing first-principles GW calculations of large model structures. A description of the valence and conduction manifolds in terms of ultra-localized non-orthogonal generalized Wannier functions permits to minimize the dimension of the basis set required for describing the space of single electron transitions. This dimension scales linearly with the size of the system. Then a real-space imaginary-time approach is used to calculate the self-energy operator in the space of Kohn-Sham eigenstates. Ultrasoft pseudopotentials are straightforwardly implemented within this scheme. We validate our approach by calculating the vertical ionization energies of small molecules and find excellent agreement with the experiment. Then we show its potentiality by addressing a model structure of vitreous silica. An overall speedup factor of up to two orders of magnitude is observed.