Jan WILHELM
BASF SE
ROM/AM - B001
Carl-Bosch-Strasse 38
67056 Ludwigshafen, Germany

Low-scaling GW calculations using Gaussian basis functions

Abstract:

The *GW* approximation of many-body perturbation theory is an accurate method for computing electron addition and removal energies of molecules and solids. In a canonical implementation, however, its computational cost is O(N^4) in the system size N, which prohibits its application to many systems of interest. I present a full-frequency *GW* algorithm in a Gaussian-type basis, whose computational cost scales with N^2 to N^3. The implementation is optimized for massively parallel execution on state-of-the-art supercomputers and is suitable for nanostructures and molecules, using either pseudopotentials or all electrons. The accuracy of the algorithm is validated on the *GW*100 molecular test set, finding mean absolute deviations of 35 meV for ionization potentials and 27 meV for electron affinities. Furthermore, the length-dependence of quasiparticle energies in armchair graphene nanoribbons of up to 1734 atoms in size is studied, and the local density of states across a nanoscale heterojunction is computed.