

GW in Gaussian Bloch Orbitals for Solids - relativistic effects, pseudopotentials, and impacts of different self-consistency cycles

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I will present recent developments in GW with Gaussian Bloch Orbitals for Solids that happened in my group. First, I will present a formulation of relativistic self-consistent GW for solids based on the exact two-component formalism with one-electron approximation (X2C1e) and non-relativistic Coulomb interactions. Our theory allows us to study scalar relativistic effects, spin-orbit coupling, and the interplay of relativistic effects with electron correlation without adjustable parameters. The simplicity of X2C1e enables the construction of higher order theories, such as embedding theories, on top of perturbative calculations.

Next, I will analyze different variants of self-consistency that can be performed in GW exclusively on the imaginary axis. To access the real axis quantities, we are using Nevanlinna analytic continuation. Within this framework, I will analyze G0W0, GW0, quasiparticle self-consistent GW scheme of Schilfgaarde, Kotani, and Faleev and QP-II scheme introduced by Kutepov, Haule, Savrasov, and Gabriel Kotliar.

Finally, I will discuss the impact of using pseudopotentials on GW calculations.