All-electron BSE@GW method for Extended Systems with Numeric Atom-Centered Orbitals

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Abstract
Green's function theory has emerged as a powerful many-body approach not only in condensed matter physics but also in quantum chemistry in recent years[1,2].We have developed a new all-electron implementation of the BSE@*GW* formalism using numeric atom-centered orbital basis sets. We present our recent developments in implementing this formalism for extended systems with the periodic boundary conditions[3]. We will discuss its implementation and numerical challenges. We will present various convergence tests pertaining to numerical atomic orbitals, auxiliary basis set for the resolution-of-identity formalism, and Brillouin zone sampling, etc. Several proof-of-principle examples will be presented to compare with other formalisms, illustrating the new all-electron BSE@GW method for extended systems.

Reference:
1. Ren, Xinguo, et al. "All-electron periodic G0W0 implementation with numerical atomic orbital basis functions: Algorithm and benchmarks." *Physical Review Materials* 5.1 (2021): 013807.
2. Yao, Yi, et al. "All-electron BSE@ GW method for K-edge core electron excitation energies." *Journal of Chemical Theory and Computation* 18.3 (2022): 1569-1583.
3. Zhou, Ruiyi, et al. "All-electron BSE@GW method with Numeric Atom-Centered Orbitals for Extended Systems." In preparation.