**One-particle Green’s functions from**

**coupled-cluster singles and doubles (CCSD) and**

**self-energy functional theory (SFT)**

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As introduced by Matsushita in this workshop, the coupled-cluster singles and doubles (CCSD) is a useful many-body approach in quantum chemistry, not based on the density functional theory (DFT). Recently there exists renewed interest for CCSD and the Green’s functions (GFs)[1] thanks to the progress of computational techniques and resources. Many-body energy spectra for realistic systems based on such explicitly correlated methods have not been, however, reported so far. We performed CCSD calculations on realistic systems, from which we calculated the GFs to analyze the electronic properties. In this presentation, we explain the details of our three recent works.

The first one[2] is the comparison between the GFs from CCSD and those from full-CI calculations for light isolated atoms. We found good agreement between the spectra calculated from the two approaches.

The second one[3] is the calculation of GFs for 3*d* transition metal isolated atoms. In addition to the CCSD calculations, we performed the electronic-structure calculations based on the self-energy functional theory (SFT)[4] for the first time. SFT is a GF-based approach, which was developed originally for solving Hubbard models. By analizing the CCSD and SFT results, we found various interesting features in those systems coming from the *d* orbitals.

The third one[5] is the calculation of GFs for realistic periodic systems. Specifically, we performed total-energy calculations and obtained the explicitly correlated band structures of C, LiH, and Be chains. We observed the satellite structures in the spectra, which do neither appear in HF nor DFT calculations.

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