**Quasiparticule spectra based on wave function theory: Application of coupled-cluster theory and self-energy functional theory**

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 Coupled-cluster singles and doubles (CCSD) is one of wave-function theories and known as a highly accurate calculation scheme in the field of quantum chemistry. Recently, the relation between CCSD and GW approximation, which is known as a well sophisticated calculation method in condensed matter physics, was clarified [1] and CCSD has get growing attention also in condensed matter physics. However, the standard CCSD scheme cannot yield quasi-particle energy spectra directly. Recently, it has been reported that by employing the one-particle Green’s function within the CCSD scheme (GFCCSD), one is capable of obtaining physical quantities including energy spectra [2]. Although the GFCCSD method has already been applied to uniform electron gases [3], there is no report of the application to realistic systems.

Fig. 1: Quasi-particle energy spectra of 1-dimensional Be chain calculated by the GFCCSD method. Fermi energy is ste to 0.

In this work, we have developed a code to calculate the quasi-particle energy spectra of isolated atoms and periodic systems through the GFCCSD method and applied it to several realistic materials for the first time [4-6]. We have also applied the self-energy functional theory to the systems for the first time and clarified the accuracy of the GFCCSD method. Consequently, we have found that the GFCCSD method is a powerful tool which enables us to calculate total energy and quasi-particle spectra self-consistently. In particular, the GFCCSD method successfully reproduces quasi-particle bands and satellite peaks at the same time as shown in Fig.1. Furthermore, we have also shown that the GFCCSD method can reproduce Mott gaps in finite systems.

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