GW + BSE calculation of RIXS spectra by the all-electron mixed basis program, TOMBO

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The initial state of X-ray emission spectroscopy (XES) and resonant inelastic X-ray emission spectroscopy (RIXS) is a highly excited eigenstate with a deep core hole after the X-ray photoelectron spectroscopy (XPS) and X-ray photoabsorption spectroscopy (XAS) processes, so that the XES and RIXS calculation offers a good example of extended quasiparticle theory (EQPT) [1] associated with many-body perturbation theory. Moreover, to overcome the basis set incompleteness problem, we adopt the all-electron mixed basis program, TOMBO, which uses both plane waves and numerical atomic orbitals as basis functions. We have successfully applied this approach in our previous XES [2] study. Here we applied the standard one-shot *GW* + Bethe--Salpeter equation (BSE) approach in MBPT to this problem on the basis of EQPT and analyze XES and RIXS energies for CH_4, NH_3, H_2O, and CH_3OH molecules.

Figure 1 shows the RIXS spectra of a CH_3OH molecule calculated by our method together with the experimental data [3]. Both results coincides very well without introducing any empirical fitting parameter.

Moreover, according to extended Kohn- Sham theory [4], we gave a justification and comment of applying the method relying on time-dependent density functional theory as well as the one-shot *GW* + BSE approach to this problem.

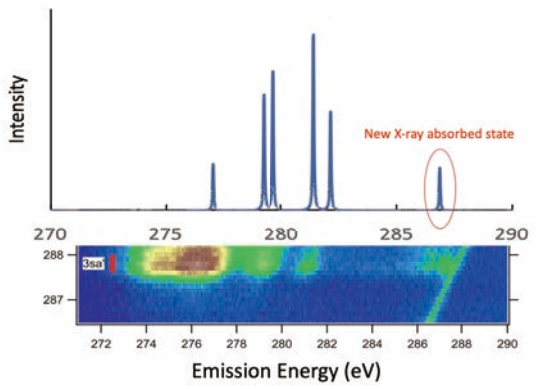

Fig. 1: Calculated (above) and experimental [3] (below) RIXS spectra of a CH_3OH molecule.

References

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