Are strong correlation and chemical realism mutually exclusive?

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Abundant work attempts to calculate realistic valence (1) and core (2,3) excitation spectra. Some of the closest agreement with experiment occurs in simple materials, e.g. semiconductors and wide-gap insulators. There, great attention is paid to the quantitative description of one-electron aspects of the calculation, such as the solution of the one-electron wave equation in the self-consistent-field calculation that underlies the many body calculation. Conversely, correlation effects on the many-body wave function are treated at a relatively simple level, such as dressing electron band energies with an approximate self-energy and considering only the effective equation of motion of a single, interacting electron-hole pair (the Bethe-Salpeter approach). While this can describe many-body effects of all electrons in a solid in a collective sense, it does not consider more elaborate processes, such as multiple excitations. On the other hand, strongly correlated systems have been treated at a more sophisticated level regarding the correlation built into the many-electron wave functions, albeit with much less chemical realism (4). In this talk, I will discuss recent work where atomic multiplet effects are built into a Bethe-Salpeter approach (5), compare this to earlier theoretical work based on an atomic model (6), and discuss how one might go beyond the two-particle limitation of the Bethe-Salpeter to treat electron correlation more adequately.

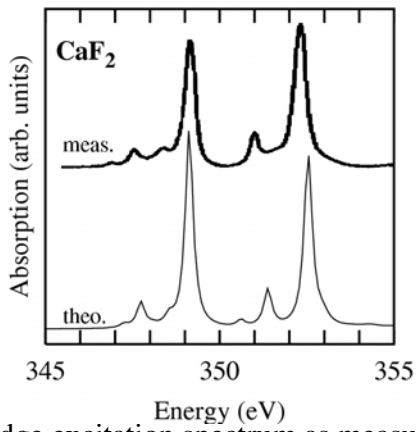

Figure 1. Calcium 2p near-edge excitation spectrum as measured and calculated.

References

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