PREDICTING CORE ELECTRON BINDING ENERGIES IN PERIODIC SOLIDS

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Theoretical methods for predicting core electron binding energies are important for the analysis of experimental results from X-ray Photoelectron Spectroscopy (XPS). The Δ-Self-Consistent-Field (ΔSCF) method is a well-known technique for calculating core electron binding energies in free molecules, but the application of this approach to periodic solids is challenging.

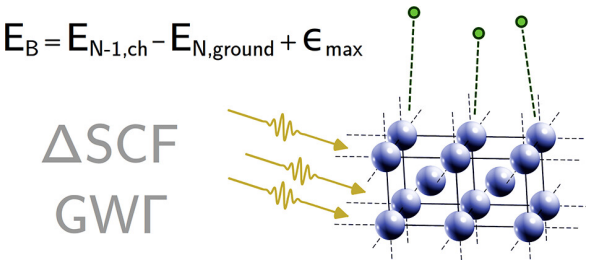

Fig.1 Graphical abstract from reference [2]. The GW and ΔSCF methods can be combined for predicting core electron binding energies in insulating solids, when the position of the valence band maximum (VBM) is used as the zero of the binding energy scale.

In this talk, recent progress in *ab initio* calculations of core electron binding energies is discussed. Solutions to problems such as charge compensation, energy referencing, and the elimination of finite size effects are examined, and an innovative approach that combines the Δ SCF method for core electron binding energies with the GW approach for predicting the position of the valence band maximum is presented. Finally, the performance of current state-of-the-art methods is evaluated by comparing the theoretical results to experimental data.

References

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2. J.M. Kahk, J. Lischner, *J. Chem. Theory Comput.* **19**, 3276 (2023)