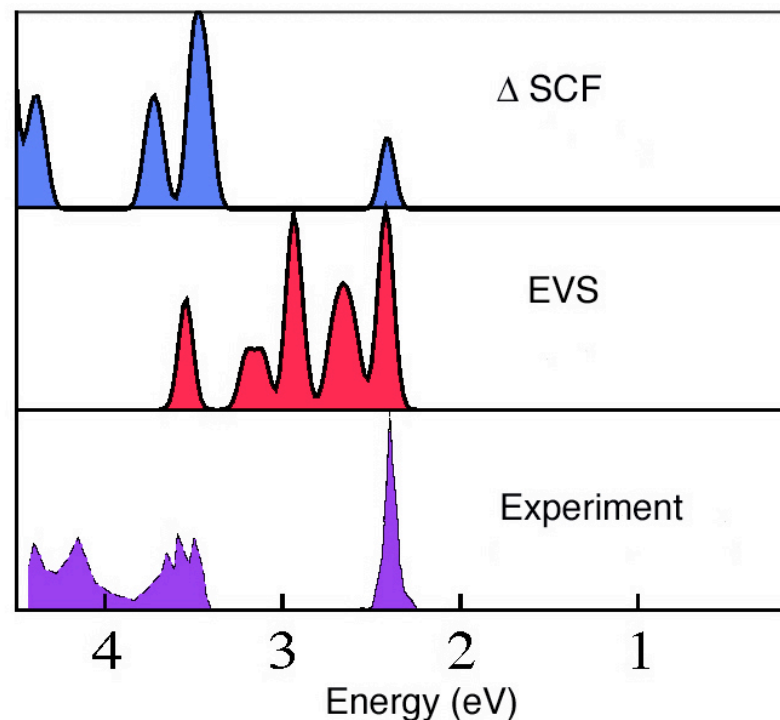


Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steve Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR- 0551195): Photoelectron Spectroscopy of Transition Metal Clusters

Clusters are materials that hold great interest both from fundamental and technological points of view. Such material can possess, for example, magnetic moments very different from the bulk phase. They can serve as a testing ground for studying the transition from atomic-like to solid-like phase as a function of the dimension of the system. A current research area is to compare calculated photoelectron spectra of clusters to experiment. A credible comparison between calculated and observed spectra will help to confirm the structure of a given cluster. We have developed new methods that yield highly accurate spectra for small clusters, provided electron-hole relaxation is included.

Ref. S. Li, M.M.G. Alemany and J.R. Chelikowsky, Phys. Rev. B **71**, 165433 (2005).



Calculated and experimental spectra for a Cu_3 anion cluster. Top panel shows the calculated spectrum allowing electron-hole relaxation. Middle panel shows the calculated spectrum using Kohn-Sham eigenvalues. Bottom panel is experiment.