

E1-30: A variational formalism to include electron correlation effects in photoionization calculations

Gunadya Bandarage^{1,2}, Robert R Lucchese²

(¹Open Univ, Nawala, Nugegoda, ²Texas A & M Univ College Station, USA)

Photoionization of core electrons of atoms and molecules is often accompanied by the simultaneous excitation of secondary electrons. In the photoelectron spectrum, the results of these shake up processes, manifest themselves as satellites. Theoretically there can be an infinite number of such satellites. However, only a few will have observable intensities. This phenomenon may be substantial in unsaturated molecules. Satellite formation is inherently a multi-electron process. Hence quantitative comparisons between theoretical and experimental cross sections for the formation of satellites is important in understanding the many-body nature of the atomic and molecular structure and the photoionization process itself.

Shake up processes are an indication of the importance of electron correlation effects in core ionization since it cannot be described by the frozen core model of the photoionization. A proper description must include the electron correlation effects even in its lowest order form. To this end, a formalism representing the electron correlation in the residual ion using configuration interaction wave functions was devised. Using an energy variational principle, a set of coupled equations were derived for the channel photoionization states. The optical potential appearing in these equations are in such a form that the usual Green's function techniques can be used to solve these equations in order to evaluate photoionization parameters.