Different routes for an accurate description of Auger-Meitner decay spectra: strategies and applications

Bruno Nunes Cabral Tenorio[1], Piero Decleva[2], Sonia Coriani[1]
[1]*Department of Chemistry, Technical University of Denmark*
[2]*Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste*
brncat@dtu.dk

Molecular Auger electron spectroscopy (also known as Auger-Meitner) is a very attractive experimental tool that encodes the electronic structure of a core-excited or core-ionized molecule into the kinetic energy of the ejected Auger electron mapping bound states to the continuum, and, essentially, probing molecular relaxation mechanisms.

We present two alternative routes to calculate Auger spectra (RAES and AES) based on

i. an explicit evaluation of two-electron bound-continuum integrals described with a multicentric B-splines basis [1], and
ii. a one-center approximation (OCA) relying on pre-calculated one-center two-electron Auger intensities instead of the exact two-electron bound-continuum integrals [2].

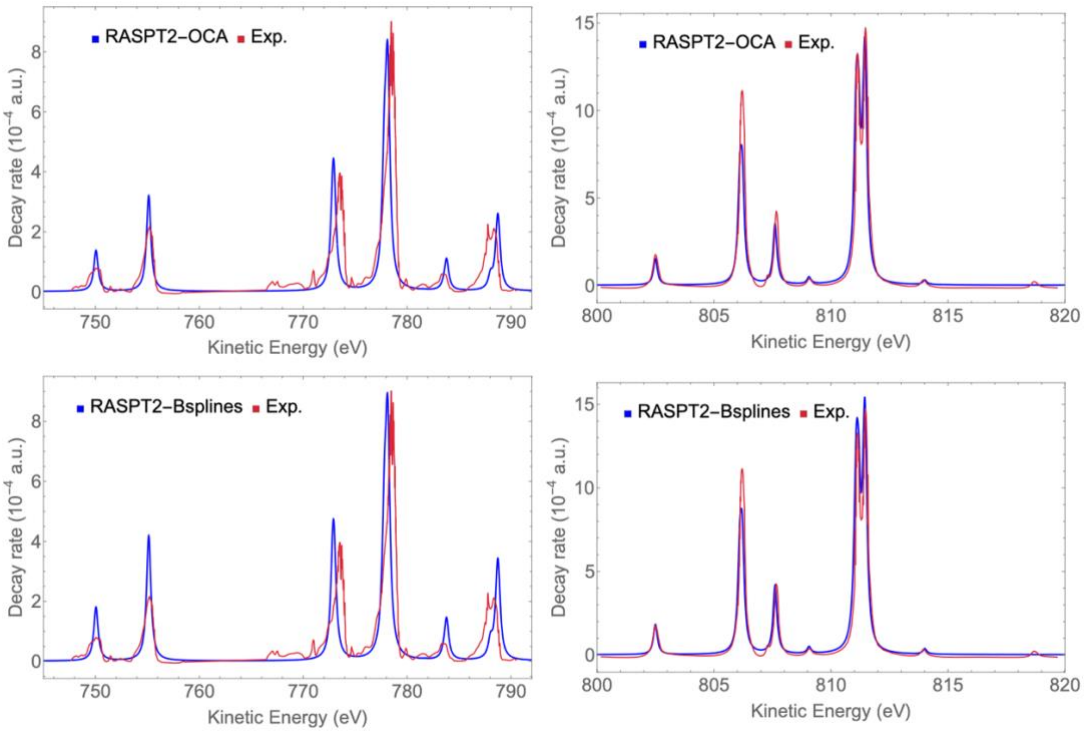

Figure 1: RAES of Ne at the 1s → 3p resonance. Calculations are in blue, and experiments are in red.

Additionally, a theoretical investigation of the time-resolved Auger decay spectra of ethylene is used to exemplify the capability of Auger spectroscopy to probe electronic and nuclear dynamics.

References

[1] Tenorio et al., 2023, in preparation.
[2] Tenorio et al., J. Chem. Theory Comput. (2022) 18, 4387-4407