Description of the *KLL* Auger-Meitner Decay Spectra of Argon following Primary and Satellite Core-Ionized States

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The *K*-edge photoelectron and *KLL* Auger-Meitner decay spectra of Argon have been investigated computationally at the restricted active space perturbation theory to the second order (RASPT2) level using biorthonormally-transformed orbital sets. Binding energies were computed for the Ar 1s primary ionization, as well as for satellite states originated from shake-up and shake-off processes. Based on our calculations, the contributions of shake-up and shake-off states to the *KLL* Auger-Meitner spectra of Argon have been completely elucidated. Our results are compared with recent state-of-the-art experimental measurements on Argon.[1]

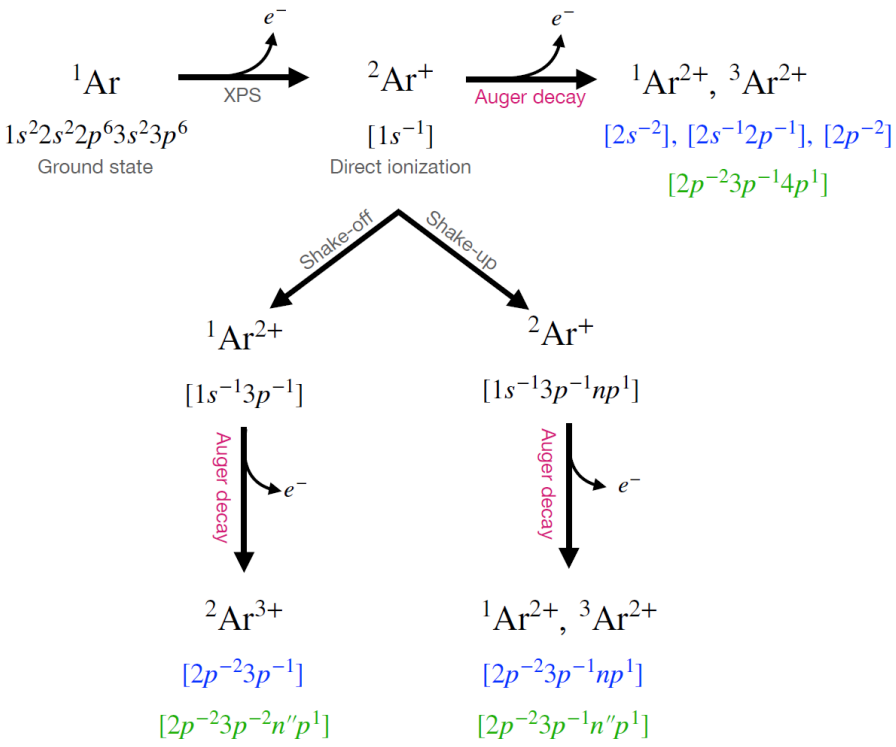

Figure 1: Schematic representation of the main Auger decay pathways of the core-ionized states. Direct Auger-decay final states and shake transitions during Auger decay are represented with blue and green, respectively.

References

[1] Püttner et al., Phys. Rev. A 102, (2020), 052832