

# Shake-up processes in Auger Cascades of Light and Medium Elements

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**Synopsis** Many-electron computations are applied to model the de-excitation of inner-shell excited atoms by a cascade of Auger decays. In particular, the effects of shake-up transitions on Auger cascades of different elements are discussed together with various theoretical models that are needed to account for the underlying electron-electron correlations.

In recent years, coincidence spectroscopy of photo and Auger electrons helped to investigate the de-excitation of atoms, molecules and solids. These techniques are, for example, used at synchrotrons to analyze the emission of multiple electrons due to Auger processes that follow the excitation or ionization of inner-shell electrons. The total kinetic energy of the emitted electrons enables one to obtain information about the spectrum and population of the final states, while the individual electron energies reveal details about the intermediate states, and therefore the decay pathways of an Auger cascade.

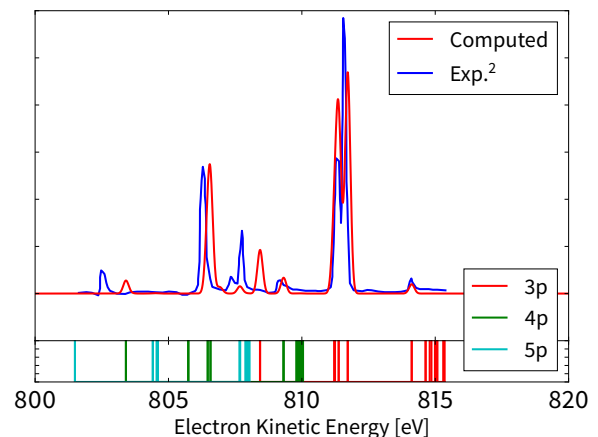
To analyze such Auger cascade processes, we have extended the RATIP program [1] to model the multiple emission of electrons after the creation of inner-shell hole states. Our studies reveal that many Auger cascades are strongly affected by shake-up (or shake-down) transitions, in which the two-electron Auger process is accompanied by an additional (de-) excitation of a valence electron. A careful treatment of the inter-electronic correlation is necessary to describe shake-up transitions in the computation of the Auger transition rates. A subsequent analysis of all possible decay paths allows to obtain quantities that are easily accessible in experiments, such as ion yields, the population of final and intermediate fine-structure levels and electron spectra.

Fig. 1 shows the electron spectrum that arises in the Auger decay of  $1s \rightarrow 3p$  resonantly excited neon to the  $1s^2 2s^2 2p^4 np$  configurations of  $\text{Ne}^{1+}$ . In this transition about 30% of the decays result in the additional excitation of one  $3p$  electron. We also show the experimental data from [2] that was obtained by a multi-electron coincidence method and that agrees very well with our computed result.

The formation of Auger cascade processes that leads to the multiple ionization of atoms after the ionization or excitation of a single inner-shell electron is in some cases strongly affected by shake-up transitions. For example, the photo ionization of a  $4p$  electron in atomic cadmium, as well as the Auger decay of this hole state, can be accompanied by an addi-

tional excitation of one  $5s$  valence electron [3]. The gain in energy due to this shake-up transition is sufficient to allow the emission of a second Auger electron. Therefore, a two-step cascade can be observed that would otherwise be forbidden energetically.

Another example for the prominent influence of shake-up transitions is the de-excitation of resonantly excited negative oxygen ions [4]. Complex electron correlation effects lead to a strong contribution of shake transitions to the total decay width. Here, the population of higher lying intermediate states even enables the occurrence of three-step Auger cascade decays that are otherwise not possible energetically.



**Figure 1.** Auger electron spectrum of the first-step decay of  $1s \rightarrow 3p$  resonantly excited neon. This spectrum is particularly influenced by shake-up transitions  $3p \rightarrow 4p$ , and is here compared with experimental data from Ref. [2].

## References

- [1] S. Fritzsche, *Comput. Phys. Commun.* **183**, 1525–1559 (2012).
- [2] Y. Tamenori and I. H. Suzuki, *J. Phys. B: At. Mol. Opt. Phys.* **47**, 145001 (2014).
- [3] J. Andersson, R. Beerwerth, et al., *Phys. Rev. A* **92**, 023414 (2015).
- [4] S. Schippers, R. Beerwerth, et al., *Phys. Rev. A* **94**, 041401 (2016).

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