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Electron transfer mediated decay of outer-valence ionised states
KIRILL GOKHBERG, VASILI STUMPF, LORENZ S. CEDERBAUM, Theoretical Chemistry, Heidelberg University — Electronically excited states of atoms and molecules embedded in an environment may efficiently decay by ionising neighbouring species in the energy or charge transfer mediated processes. The energy transfer driven interatomic Coulombic decay (ICD) has been shown to proceed on a fs time scale in weakly bonded systems upon the production of a localised electronic excitation. Related electron transfer mediated decay (ETMD) is usually a slower process and becomes an important relaxation pathway whenever ICD channel is unavailable. In this talk we show that this situation is realised for singly and multiply outer-valence ionised atoms in a medium leading to unexpected physical effects. In particular, we demonstrate that ETMD provides an efficient and general neutralisation pathway for multiply charged ions produced via Auger decay in an environment. As an example we show the results of an ab initio study of the $NeKr_2$ cluster following the Auger decay of 1s vacancy of Ne. We also discuss how the single photon double ionisation efficiency can be dramatically enhanced in a medium due to ETMD. As an example we show that the double ionization cross section of Mg in MgHe cluster becomes three orders of magnitude larger than the respective cross section of the isolated Mg atom.

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