Interatomic Coulombic Decay of HeNe dimers after ionization and excitation of He and Ne

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Synopsis We present a detailed study of Interatomic Coulombic Decay (ICD) in Helium Neon dimers after ionization and excitation of the helium or the neon atom. Depending on the initial excited state direct ICD or exchange ICD is the preferred route of dexcitation.

After Interatomic Coulombic Decay (ICD) was predicted in 1997 by L. S. Cederbaum *et al* [1] and confirmed experimentally in 2004 [2-4] it was the subject to a plethora of studies covering several atomic and molecular systems. As a follow-up study to [5] we investigate ICD after shake-up ionization in HeNe dimers identifying all involved decay channels, intermediate states and decay processes.

Upon irradiation by synchrotron radiation at Beamline U125-2_SGM from the photon source BESSY II an intermediate excited $HeNe^{+*}$ state is populated. The system decays into the $He^{+}(1s^{-1}) - Ne^{+}(2p^{-1})$ final state via either direct or exchange ICD depending on that intermediate states parity. Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS) [6] was used to detect all reaction fragments in coincidence and measure their initial momenta.

As direct ICD involves a virtual photon to transfer the excess energy its R-dependency goes with $1/R^6$ and it is forbidden for intermediate states in which either He has *gerade* parity or Ne has *ungerade* parity.

On the other hand, for direct ICD an overlap of the electron orbitals between He and Ne is needed. Therefore, its R-dependency is exponential and it becomes dominant for smaller internuclear distances.

Figure 1 depicts the experimental yield as function of electron energy and kinetic energy release (KER) of the ions. The latter is equivalent to the inverse internuclear distance in atomic units. Various diagonal and horizontal structures are visible corresponding to ICD and photoelectrons that are emitted during the decay process starting from different intermediate excited states.

In good agreement with previous work [7] direct and exchange ICD are observed in different regions of KER. Large internuclear distances correspond to the case of direct ICD and small distances are related to exchange ICD.

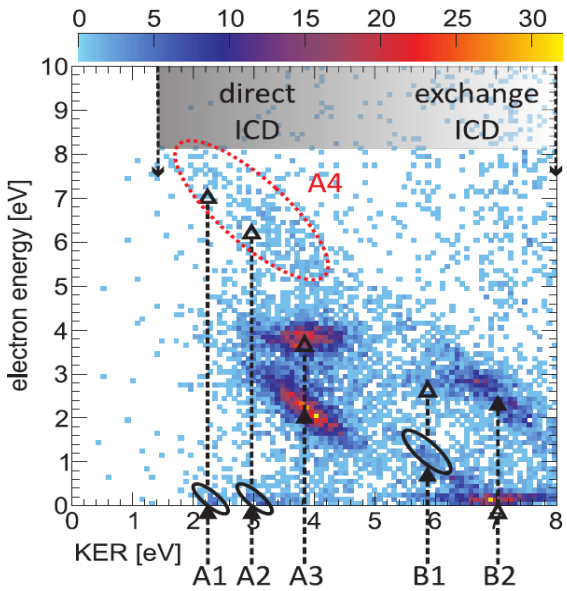

Figure 1. Electron energy distribution in dependence of the recoil kinetic energy release.

References

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