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Interatomic Coulombic decay mediated by ultrafast superexchange energy transfer

Tsveta Miteva[1], **Sevan Kazandjian**[1], **Premysl Kolorenc**[2], **Petra Votavova**[2] and **Nicolas Sisourat**[1]
[1]Sorbonne University, France
[2]Charles University, Czech Republic

Inner-valence ionized states of atoms and molecules live shorter if these species are embedded in an environment due to the possibility for ultrafast de-excitation known as interatomic Coulombic decay (ICD). In this process the initially excited species de-excites by transferring its energy to a neighbor and ionizing it within femtoseconds. The ICD lifetime, or going from the time to the energy domain, the ICD width, depends on the distance between the interacting monomers. At large interatomic separations, the process can be viewed as an exchange of a virtual photon between the monomers and thus, the decay width displays a $1/R^6$ dependence on the distance. In this work we show that the lifetime of the ICD active states decreases further when a bridge atom is in proximity to the two interacting monomers. This novel mechanism, termed superexchange ICD, is driven by the efficient transfer of excitation energy via virtual states of the bridge atom. As a showcase system we consider the NeHeNe trimer. The decay widths of the $Ne_2^+(2s^{-1})\ ^2\Sigma_g^+$ state in the presence of He and in the isolated dimer were computed using the Fano-CI method. We demonstrate that the decay width of the $Ne_2^+(2s^{-1})\ ^2\Sigma_g^+$ resonance increases 6 times in the presence of a He atom at a distance of 4 Å between the two Ne atoms. Using a simple model, we provide a qualitative explanation of the superexchange ICD and we derive an analytical expression for the dependence of the decay width on the distance between the neon atoms.

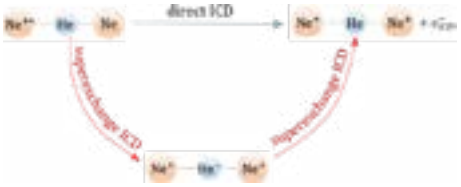

Figure 1: Schematic representation of the superexchange ICD process in NeHeNe trimer

Recent Publications

1. L S Cederbaum, J Zobeley and F Tarantelli (1997) Giant intermolecular decay and fragmentation of clusters. Phys. Rev. Lett. 79:4778.
2. R Santra, J Zobeley and L S Cederbaum (2001) Electronic decay of valence holes in clusters and condensed matters. Phys. Rev. B 64:245104.
3. V Averbukh, I B Müller and L S Cederbaum (2004) Mechanism of interatomic Coulombic decay in clusters. Phys. Rev. Lett. 93:263002.
4. T Miteva, S Kazandjian and N Sisourat (2017) On the computations of decay widths of Fano resonances. Chem. Phys. 482:208.

Biography

Tsveta Miteva received her bachelor's and master's degree in chemistry from Sofia University St. Kliment Ohridski, Bulgaria. She has her research focused on the theoretical description of electronic decay processes in atomic and molecular systems. In order to understand and model these ultrafast processes, she developed and implement original numerical tools. Another part of her research focuses on the electronic relaxation mechanisms following X-ray absorption in aqueous salt solutions.

miteva.tsveta@gmail.com