Molecular dissociation after Resonant Auger decay in O2 and N2

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When an electron is resonantly excited from a core orbital to a Rydberg one in a molecule, complex multistep processes at different time scale are triggered. By using a high-resolution energy-resolved coincidence between Auger electron and ions, we identified the sequences of processes following the spectator Auger decays induced by K-shell excitation in O2 and N2 molecules.

Spectator Auger decay happens after O $1s \rightarrow (^4\Sigma_u^-)4p\sigma$ excitation, then the majority of O_2^+ states dissociate into several limits with complex crossings between potential-energy curves. After the molecular dissociation is finished, the generated fragments can further decay either by fluorescence emission or by autoionization. Interestingly, some electrons are always emitted after molecular dissociation. Weak dissociation limits that contain only valence electron are also identified. It indicates that the electron orbital size tends to be conserved during the dissociation process. These weak features are suggested to be created by the Rydberg-valence mixing between the molecular spectator Auger final state and the very dissociative molecular cationic states without the Rydberg electron.

Vibronic coupling can happen during dissociation. We identify the resonant Auger decay channels that lead to the lowest dissociation limit after the excitation N 1s $\rightarrow \pi_g^*$ in N2 molecule. From the kinetic energy release spectra of these channels at vibrational quantum number v = 0, 1, and 2 in the excitation, we give a clear proof of the vibronic coupling between the D $^2\Pi_g$ and 2 $^2\Pi_g$ states, which is not clear in previous papers.