Many-body molecular fragmentation: beyond the Born-Oppenheimer and the independent electron approximations

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Ionic fragments originating from molecular bond cleavage are highly reactive and very efficient in modifying their microscopic surroundings, occurring in several environments where molecules are subjected to ionizing radiation (electrons, heavy ions or photons) such as radiation therapy, planetary atmospheres, ionospheres and magnetospheres. If the ionized electron is removed from the core or from the inner valence molecular orbital, a complete fragmentation can occur. This removal results in a fast (fs time-scale) electron and nuclear rearrangement, where the electron correlation is dominant, and the independent electron approximation is not applicable. Simultaneously, there is a strong induction of nuclear movements associated with this fast electronic rearrangement and the Born-Oppenheimer approximation also breaks down. This scenario makes the double excitation mechanisms, such as shake-off, Auger, shake-up and satellite states formation, the main actors in the energy redistribution process that will result in the simultaneous disruption of several chemical bonds resulting into the various final products observed from the fragmentation. The theoretical description of this ultra-fast phase of redistribution of energy is virtually non-existent, even for light molecules. In this talk it will be presented how some experimental signatures of these complex mechanisms can be identified and quantified. As an example, the geometrical rearrangement occurring along with the full fragmentation of water molecule induced by electron impact, and giving rise to the O$^+$ cation, will be discussed.