

Ultrafast dynamics of XUV induce multielectronic excited states in PAH molecules

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The relaxation dynamics of Polycyclic Aromatic Hydrocarbon (PAH) molecules excited by XUV photons has a clear importance in astrochemistry due to the abundance of such molecules and photons in space and more precisely to assign the diffuse interstellar bands (DIBs). Photon with energy greater than the ionization potential can produce excited states, where electron correlation plays a crucial role. The present work shows how these states evolve in the early time that follows the excitation.

With the emergence of the XUV-IR pump-probe experimental scheme, such dynamics can be studied with temporal resolution. In our experiment, first a XUV pulse (15-40 eV) of few tens of femtoseconds (produced by High Harmonic Generation) is used to excite the molecule in multielectronic states. Then a femtosecond (800 nm) pulse probes the decay process through a few photon ionization of the excited state. Time dependent ion yield is measured.

Non-adiabatic relaxations of the excited PAH molecules are observed within the first few tens of fs. Our results are supported by high level multielectronic and non-adiabatic theoretical description showing that correlation and vibronic couplings are responsible of this mechanism.

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