

# Ultrafast Non-adiabatic Relaxation in XUV-excited Molecules

Alexander I. Kuleff

*Theoretische Chemie, PCI, Universität Heidelberg,  
Im Neuenheimer Feld 229, D-69120 Heidelberg, Germany  
alexander.kuleff@pci.uni-heidelberg.de*

Exposing molecules to XUV radiation populates typically highly-excited cationic states that triggers complex ultrafast dynamics in which both the electron and the nuclear motions are strongly coupled. A fully quantum description of these dynamics in small polycyclic aromatic hydrocarbons (PAH) will be reported and compared to time-resolved experimental results [1,2]. It will be shown that the non-adiabatic relaxation dynamics gets slower the closer the initial excitation is to the double-ionization threshold, and also when increasing the size of the system. Moreover, it will be demonstrated that the dynamics in these energy range is governed by the so-called correlation bands, features created by the strong electron correlation in the inner-valence, and a simple electron-phonon scattering model may be used to explain and predict the relaxation dynamics of whole classes of molecules.

## References

- [1] A. Marciniak, *et al.*, Nature Commun. **6**, 7909 (2015).
- [2] A. Marciniak, *et al.*, Nature Commun. **10**, 337 (2019).