CFEL SCIENCE

SEMINAR

23th May 2018 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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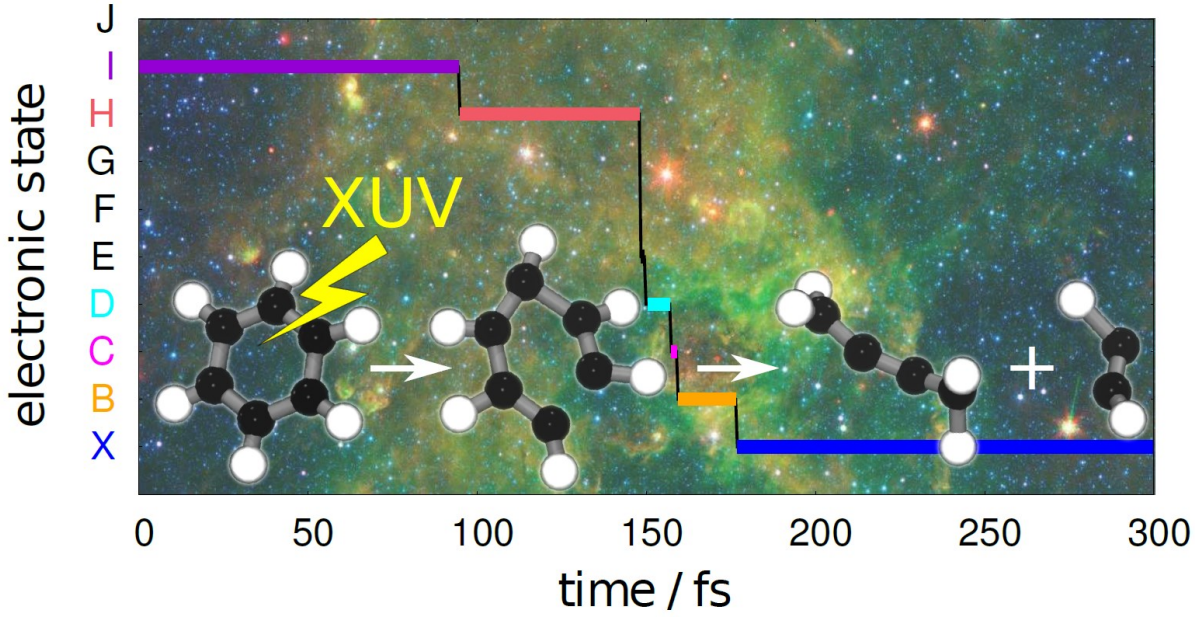
Ultrafast fragmentation dynamics of the benzene radical cation

Certain infrared emission bands observed from outer space are attributed to the presence of polycyclic aromatic hydrocarbons (PAHs) in the interstellar medium (ISM). Our understanding of the role of XUV-induced chemistry in the ISM and from complex molecules is an essential first step into unraveling the evolution of biological complexity in the most inhospitable regions of the universe.

However, it is challenging to simulate the XUV photochemistry of PAHs as one has to deal with a broad range of excited states, as well as several nuclear degrees of freedom, and a multitude of fragmentation channels. I will discuss the possibility of utilizing a Koopmans' theorem based electronic structure approach to study two aspects of the ultrafast XUV photochemistry of the prototype benzene cation: (i) the time-resolved relaxation of the electronically excited states and (ii) the time-resolved fragmentation dynamics. The theory is based on ab initio classical trajectory calculations within the fewest switches surface hopping (FSSH) scheme.



Host: Robin Santra – CFEL-DESY Theory Division