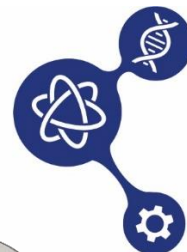


# Seminario de Química Física



Martes 23 de julio de 2024 – 11:30 h



Salón de Actos de la Biblioteca

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## Nonadiabatic Reaction Dynamics of Polyatomic Molecules (or Anions): Role of the Electron in the (Non)Valence Orbitals

Non-valence bound state (NBS) of the anion is ubiquitous in nature and plays the essential role of the doorway into the anion physics and chemistry. Here, the state-specific chemical dynamics of the metastable NBSs using the picosecond time-resolved pump-probe spectroscopy on the cryogenically cooled anions using the velocity-map ion/electron imaging technique has been utilized to unravel the nature of the mode-dependent dynamic behavior of the NBS in terms of the autodetachment and/or concomitant fragmentation reactions. The autodetachment rate of the NBS has been precisely measured in a state-specific way for various chemical systems of the phenoxide, 4-cyanophenoxide, or *o*- (*m*- or *p*-) halogen substituted phenoxides. Fermi's golden rule is found to be extremely helpful for the rational explanation of the experiment, and yet the much more sophisticated theoretical model was required for the quantitative analysis. For (*ortho*-, *meta*-, or *para*-) iodophenoxides, the C-I bond rupture (giving the I fragment at the asymptotic limit) has been found to be mediated by Feshbach resonances of the NBS, providing the foremost evidence for the dynamic doorway role of the NBS in the anion chemistry and physics. Autodetachment and the NBS-VBS (valence bound state) transition processes are kinetically competitive, promising the quantum mechanical control of the anionic reaction. Regarding the nonadiabatic transitions, the structure of the conical intersection and nearby potential gaps along the multidimensional potential energy landscape govern the dynamic outputs. The experimental perspective on the conical intersection dynamics will be also given if time is allowed.

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