

PTPC2019

Contribution ID: 2

Type: **not specified**

Photoionization and Photoelectron Spectroscopy of Biradicals

Friday, 11 January 2019 09:55 (25 minutes)

Biradicals are molecules with an electronic structure that is characterized by two unpaired electrons in degenerate or near-degenerate molecular orbitals. Their chemical and physical properties differ significantly from those of closed-shell molecules due to the interactions between the energetically close-lying states that result from the degenerate molecular orbitals. Biradicals play an important role in the chemistry of reactive environments like combustion engines, the atmosphere or interstellar clouds. Furthermore electronic states with a biradical character are key intermediates in the formation of light-emitting states in optoelectronic materials. It is therefore of relevance for many areas of chemistry and physics to understand and correctly describe the structure and dynamics of biradicals and molecules with biradicalic electronic states. In my talk I will present recent work on the photoionization of biradicals, including molecules like diborene and ortho-benzyne. The experimental work is accompanied by high-level computations.

Primary author: FISCHER, Ingo (Universität Würzburg)

Presenter: FISCHER, Ingo (Universität Würzburg)

Session Classification: Photoionization spectroscopy I