29th Summer School and International Symposium on the Physics of Ionized Gases

Aug. 28 - Sep. 1, 2018, Belgrade, Serbia

CONTRIBUTED PAPERS

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ABSTRACTS OF INVITED LECTURES, TOPICAL INVITED LECTURES, PROGRESS REPORTS AND WORKSHOP LECTURES

Editors:
Goran Poparić, Bratislav Obradović,
Duško Borka and Milan Rajković

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PREFACE

This publication contains the contributed papers and abstracts of Invited Lectures, Topical Invited Lectures, Progress Reports and Workshop Lectures that will be presented at the International Symposium on the Physics of Ionized Gases 2018. This is the 29th of a series of events which reflect the progress in this challenging field of science. The event is organized by the Vinča Institute of Nuclear Sciences in Belgrade and Serbian Academy of Sciences and Arts, with the support of the Ministry of Education, Science and Technological Development of the Republic of Serbia.

The aim of this book is to present new results in the fundamental and frontier theories and technology in the area of general plasma physics (including astrophysical and fusion plasmas), atomic collision processes and particle and laser beam interactions with solids. Also, the presented results and lectures of the 3rd Workshop on X-ray and VUV interaction with Biomolecules in Gas Phase - XiBiGP are also included.

Herein, the Editors would like to thank the authors and reviewers for their support of this event and to wish all participants a pleasant and productive stay in Belgrade. We are grateful to the Serbian Academy of Sciences and Arts for their long term commitment to support this event as well as the Serbian Ministry of Education, Science and Technological Development for their continuing help. We also acknowledge the support of the open access journal "Atom"

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COMPUTATIONAL TOOLS FOR STUDYING X-RAY – MOLECULE INTERACTIONS: PHOTOFRAGMENTATION OF HALOTHANE

M. Radibratović[1], S. D. Tošić[2], M.C. Castrovilli[3], J. Chiarinelli[3,6], P. Bolognesi[3], L. Avaldi[3], R. Richter[4], M. Coreno[3,4], B. P. Marinković[2] and M. K. Milčić[5]

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Halothane ($C_2HBrClF_3$), one of the most commonly used halogenated anesthetics, play a significant role in the destruction of the earth's ozone layer [1]. Photofragmentation experiments in the VUV and soft X-ray energy regions performed at Elettra synchrotron have shown that the mass spectra of halothane is dominated by lighter mass fragments. To explain the experimental findings extensive computational studies were conducted. Low level, but fast and accurate self-consistent charge density-functional tight-binding (SCC-DFTB) theoretical method was employed to simulate the fragmentation of singly and doubly charged halothane ions from their ground state electron configurations at different temperatures. A number of fragmentation paths were simulated producing almost all fragments found in the mass spectra. For the main fragmentation pathways, the minima and the transition states on the potential energy surface were described with more accurate computational methods.
In order to obtain a better insight in the photofragmentation pathways nonadiabatic dynamics simulations were conducted using trajectory surface hopping method (Newton-X program), combined with TD-DFT (Gaussian09) and MCSCF (Columbus) electronic structure methods. The results have shown the relevance of the cation excited states in the photofragmentation processes.

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