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Editorial

Dynamics of molecular systems*

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1 Introduction

The present edition of MOLEC, the XXI European Conference on the Dynamics of Molecular Systems, MOLEC 2016, held in Toledo (Spain), has attracted 107 participants from more than 20 countries, both European and non-European ones. The scientific program was structured in 15 thematic sessions that included 46 lectures (15 Plenary, 15 Invited, and 16 Oral Contributions). The most recent experimental and theoretical advances in different areas of Molecular Dynamics were presented in those lectures. More specifically, the program covered the areas of molecular collisions, electronic structure calculations, ultracold atoms and molecules, molecular dynamics in gas, condensed phases, and interfaces, control of molecular processes, photon–matter interactions, astrophysics, astrochemistry, and atmospheric chemistry. The meeting also scheduled two poster sessions where 67 poster contributions were presented, allowing for excellent opportunities for additional fruitful discussions.

The XXI edition happily coincided with the 40th anniversary of the MOLEC conference, and this event was celebrated with a special opening session. In this opening session two Plenary lectures were scheduled to be delivered by the founders of the MOLEC conference in 1976, Professors Jan Peter Toennies and Franco Antonio Gianturco, as a tribute to them. In the conference the traditional MOLEC Senior Prize was awarded to Professor Dieter Gerlich to honor his outstanding contributions. For the occasion of the 40th anniversary of the conference, a new MOLEC prize was established, namely the Zdeněk Herman Young Scientist Prize, which was awarded to Professor Sebastiaan Y.T. van de Meerakker. The XXI edition of the conference was dedicated to the memory of Professor Ahmed Zewail, who sadly passed away last August 2nd, 2016, just about a month before MOLEC 2016 was celebrated. Professor Zewail, who was awarded the Nobel Prize for Chemistry in 1999, made outstanding contributions to the field of Molecular Physics and Chemical Physics, which are the fields of the MOLEC conference.

2 Progress in molecular dynamics

The present topical issue on Dynamics of Molecular Systems includes 12 contributions that present state-of-the-art experimental and theoretical advances on different areas of Molecular Dynamics reported by leading research groups. They cover areas such as spectroscopy, photodissociation, and reaction dynamics of neutral and ionic molecular and cluster species.

Schaupp et al. [1] reported an investigation of the correlated electron-nuclear dynamics in a dissociating model system, using both classical and quantum mechanical methodologies. A study of the relaxation dynamics of the internal rotational energy of the diatomic ions para-H_2^+, orto-D_2^+, and HD^+ in collision with cold He atoms has been presented by Hernández Vera et al. [2]. A comprehensive analysis of the vibrational structure of the CO_2 system applying a polyad-preserving algebraic approach was presented and discussed by Bermudez-Montaña et al. [3]. Zhang et al. [4] have reported a combined experimental and theoretical study of the dissociative ionization and Coulomb explosion of CH_3I when intense femtosecond laser fields are used. The relationship between the conditional quasi-exact solvability of the planar pendulum eigenproblem and the topology of its eigenenergy surfaces has been examined and discussed by Becker et al. [5]. The structural and spectroscopic characterization of various isotopologues of 2-hydroxyacetonitrile with ab initio methods has been reported by Dalbouha et al. [6]. Chang et al. [7] have shown theoretically the possibility of control

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of the bond distance in the RbCs dimer by applying a chirped laser pulse. A theoretical study of the reactive pathways leading to hydrogen and carbon removal when F atoms react with organosilicate glass low-κ films has been reported by Voronina et al. [8]. The nature of non-covalent interactions in isolated amino acids have been analyzed in an experimental work reported by González et al. [9]. The transport of low energy electrons in furfural molecules has been investigated experimentally and reported by Lozano et al. [10]. Baturo et al. [11] reported an experimental study on the predissociation of the Rg-I_2 (Rg = rare gas atom) van der Waals complexes in their ion-pair excited electronic state. Finally, details on a new apparatus to investigate the visible and near infrared fluorescence spectroscopy of electronically excited helium over a wide range of pressures and temperatures in gaseous and liquid phases have been presented by Shiltagh et al. [12].

3 Summary

We note that, although all the papers included in this topical issue are related to MOLEC 2016, they were submitted after the conference was celebrated, and have all passed the full editorial treatment and evaluation according to the high standards of the journal. This issue contains high quality contributions that can help and motivate future works. We thank all the contributors of this issue for their participation. We also thank the support provided by the editorial staff of the journal during the review and edition process. The organizers of MOLEC 2016 hope that this conference provided a fruitful venue for the advance of Molecular Dynamics.

Author contribution statement

All the authors have contributed to the design and writing of this Editorial.

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