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EDITORIAL

Special Issue: CAMOP–MOLEC XV

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On behalf of the organizing and international scientific committee of MOLEC XV

The advances in recent years in the field of molecular dynamics are numerous and impressive. In sophisticated experimental and theoretical studies it is nowadays possible to steer chemical reactions with quantum-number-prepared molecules, to study reaction products fully state-specifically, and to derive accurate potential energy surfaces with the goal of determining the pathways along which molecular interaction can take place. Both experimental and theoretical techniques have rapidly improved, and our understanding of the dynamical nature of chemical processes is continuously growing.

In this special issue of CAMOP/*Physica Scripta* we have tried to present a snapshot of the state-of-the-art in the field of molecular dynamics. It contains a collection of papers submitted in association with the most recent MOLEC meeting (MOLEC XV) held in September 2004 in Nunspeet, The Netherlands. This biannual meeting started in 1976 in Trento and was subsequently organized in Brandbjerg Højskole (Denmark, 1978), Oxford (UK, 1980), Nijmegen (The Netherlands, 1982), Jerusalem (Israel, 1984), Aussois (France, 1986), Assissi (Italy, 1988), Bernkastel-Kues (Germany, 1990), Prague (Czech Republic, 1992), Salamanca (Spain, 1994), Nyborg Strand (Denmark, 1996), Bristol (UK, 1998), Jerusalem (Israel, 2000) and Istanbul (Turkey, 2002). Within the philosophy of CAMOP we have asked invited speakers to report on outstanding problems in their particular field. This comprises discussion of open questions, important applications, new theoretical and experimental approaches and also predictions of future developments. A good comment, in addition to being an authoritative contribution of an acknowledged expert, should also be readable by the non-expert and we have taken special care that the work presented here is introduced in an understandable way and has been placed within the context of accessible literature for the interested reader.

The sequence of 16 papers that is presented in this issue is arranged according to three main topics that form a focus within the field and can be roughly summarized as induced chemical (intermolecular) dynamics, molecular spectroscopy/theory, and photo-induced uni-molecular (intramolecular) dynamics.

The issue opens with a contribution by the MOLEC XV award winner Levine and his co-workers (the paper by Kornweitz *et al*) in which they speculate on the possibility of probing electronic rearrangement in a chemical collision using light emitted during the very collision. Banares and co-workers continue with an overview on what is and what is not understood about the dynamics of the 'most simple reaction' $H + H_2$ and prospects for future research of this prototypic system are presented. The effect of molecular structure on chemical dynamics is discussed by Pearce *et al* on the example of HCl originating from Cl atoms reacting with different organic ethers. Stereodynamical effects are discussed by Cappelletti and co-workers starting from collisional alignment in supersonic seeded molecular beams with applications ranging from (in)elastic events to selective surface scattering experiments. A laboratory controlled study of chemical reactions under interstellar conditions using temperature variable multi-electrode traps is reviewed by Gerlich and Smith. Eritt *et al* discuss a technique capable of studying the interaction of electrons with size selected molecular ions and results are presented for the electron detachment of C_n- and Al_n-clusters. Ultrafast dynamical events at a conical intersection are discussed in a theoretical study by Burghardt *et al* and the experimental tools to study electron

dynamics are presented by Vrakking in a contribution on direct and indirect methods to generate attoseconds.

In four spectroscopic and theoretical contributions the latest findings are presented in interpreting and understanding complicated molecular spectra. Meerts and Smit introduce a powerful numerical assign and analysis method based upon genetic algorithms and its performance is demonstrated on the example of dense spectra of (complexed) aromatic species. Interaction potential surface calculations of rare gasses with halogens in van der Waals complexes are described by Delgado-Barrio and co-workers, and Tennyson discusses new theoretical techniques based on the use of the variational principle to guide the spectral assignment of complicated water spectra, e.g. at very high temperatures. Finally, Okumura and co-workers present NIR spectra of NO_3 and in combination with new calculations these shed light on how to interpret vibronic couplings in this interesting system.

The last section of this issue comprises fragmentation and photo-dissociation studies. Rubio-Lago *et al* discuss methods to produce high-density spin polarized hydrogen following photodissociation experiments. The photodissociation of HCl and Cl_2 is taken as an example by Balint-Kurti *et al* to demonstrate how amplitudes and phases of the photofragmentation matrix elements are derived from experimental measurements. Directional dynamics in photodissociation processes and the derivation of molecular frame properties are discussed in detail by Van den Brom *et al* using laboratory oriented molecules. And the issue closes with a contribution by Chambreau *et al* on different reaction mechanisms in the photodissociation of formaldehyde into H_2 and CO.

Coming to the end of this editorial, we wish to thank all the authors who participated with their contributions in this issue. It shows what is possible nowadays in the field of molecular dynamics and where things are heading in the near future. We thank *Physica Scripta* for providing us with the platform for this Special Issue, and we wish you, dear reader, many new insights!