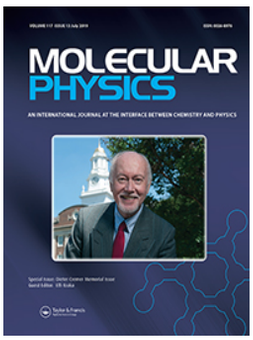

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Special issue: atoms, molecules, and clusters in motion

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EDITORIAL

Special issue: atoms, molecules, and clusters in motion

The majority of the contributors to this Special Issue come from two, considerably overlapping communities. The first community includes the participants of the 3rd AMOC international conference (http://kkrk.chem.elte.hu/amoc), which took place in Budapest between April 16–19, 2018 (the first two meetings in this series were held in Paris and Madrid in 2012 and 2015, respectively). The second community is that of a COST action (CM1405), MOLIM: Molecules in Motion. The MOLIM action (http://cost-molim.eu) had its 3rd General Meeting in Budapest following the AMOC meeting. Both of these communities deal with the motions of nuclei in a very broad and general sense and include both experimentalists and theoreticians (molecular physicists and quantum chemists).

Both the AMOC conference series and the MOLIM community do stress action building, with a special emphasis on the involvement of early career investigators (ECIs). Both communities are centred around leading European research laboratories with strong ties to groups outside of the EU. As a result, most of the contributors to this Special Issue are from the EU but there are two articles from authors from China and one from Japan and there are several contributions from ECIs.

The Special Issue at hand discusses a number of different approaches to overcome the difficulties associated with the experimental and computational treatment of anharmonic and nonrigid nuclear motions in simple and complex quantum systems. As usual in the field of nuclear motions, one has to consider model systems to improve our understanding of small complex molecular systems and larger molecules and clusters. As it is clear from this Special Issue, there are a large number of still unsolved, challenging problems to tackle in molecular sciences not only for large molecules (*e.g.*, drug isomers [1] and sensors [2,3]) but also for small molecules (*e.g.*, diatomics). To this end, we learn how H atoms escape confinement [4], about the use of the Deng-Fan potential energy curve to obtain X-H stretching intensities [5], the relation of highly excited molecular states to ideal-gas partition functions [6], as well as new facts about the diatomic molecules C_2 [7] and KS [8]. Triatomic systems treated in this Special Issue include H_3^+ [9] and Ca^+-Ar_2 [10], for which accurate potential energy surfaces have been developed. We also learn how to understand certain characteristics of the motions of quantum systems from variationally computed wavefunctions [11] and about the nuclear dynamics of the CH_4-Ar complex [12], formic acid [13], heavy protonated noble-gas species [14], the methanol cation under the influence of strong laser fields [15], and nitrosamine [16]. One of the goals of this Special Issue has been to address the treatment of nuclear motions of clusters. Related applications include, for instance, the accurate description of highly excited (electronic as well as vibrational and rotational, bound and unbound) states of molecules and weakly bound aggregated systems as well as the dynamics of molecules adsorbed on nanostructures [17–19].

As organisers of the above-mentioned two scientific conferences, it gives great pleasure for us to see several contributions to these meetings appearing in this Special Issue dedicated to nuclear dynamics. We do appreciate all the work the authors put into preparing their manuscripts. Needless to say, the papers went through a rigorous reviewing and editorial process. It is hoped that *Molecular Physics* continues to serve our community and that our community will help *Molecular Physics* to achieve its goal of publishing cutting-edge experimental, theoretical, and computational results.

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