

Atomic cluster collisions: ISACC-2015 (7th International Symposium)*

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Abstract. The ISACC 2015 brought together nearly a hundred scientists in the field of atomic and molecular cluster physics from around the world. We deliver the Editorial of a topical issue compiling/presenting original research results from some of the participants on both experimental and theoretical studies involving research areas from small clusters to extended molecular systems in the field.

The idea of this Topical Issue was to collect recent results which have been produced in this area by the international community and, therefore, to provide a current state-of-the-art description of what is being done in the field of structure formation and dynamics of nuclear, atomic and molecular clusters, nano-objects, ensembles of nanoparticles, nanostructures, biomolecules and biomolecular systems. Although the current Topical Issue is not a collection of conference proceedings, the participants of the 7th International Symposium “Atomic Cluster Collisions” (ISACC 2015) made the contribution by submitting their novel and original results.

Since 2003, the ISACC meetings [1–7] promote the growth and exchange of scientific information on the structure, properties and dynamics of complex nuclear, atomic, molecular, cluster, nanoscopic and biological systems studied primarily by means of photonic, electronic, heavy particle and atomic collisions. In ISACC 2015, [7] held at Madrid on the 18–21 July as a satellite of the ICPEAC 2015¹, particular attention was devoted to dynamical phenomena, many-body effects taking place in clusters, nanostructures, molecular and biological systems, which included problems of fusion, fragmentation, collective electron excitations, phase transitions, and radiation damage among several exciting issues. Both experimental and theoretical aspects of cluster physics uniquely placed between nuclear physics on one hand and atomic,

molecular and solid state physics on the other hand were the subject of the symposium.

This themed issue, as well as the ISACC 2015 Symposium, attends to a wide range of techniques for spectroscopy and collision dynamics covering an ample field of phenomena. Techniques vary from ab initio calculations and new theoretical models to state-of-the-art laboratory methodologies. Thus, this publication brings together theoretical and also experimental articles. Experimental techniques, rapidly becoming more accurate, demand state-of-the-art theoretical methodologies for the interpretation of the measurements. The studied species show sizes and varied compositions from small- to large sized systems. Studies encompass from tri- and tetra-atomic systems and their corresponding clusters containing a large number of units, up to biological species with scores of atoms. Briefly, sessions included topics (see Fig. 1) on many different types of clusters and processes, e.g. weakly bound van der Waals (vdW), metallic [8–10], nanodroplets [11–13], fullerenes [14,15] PAHs (Polycyclic Aromatic Hydrocarbons)/carbon-layered [16–19], water and mixed-water clusters [20–24] and clathrates [25,26]; spectroscopic and collisional processes of excited molecules in the gas phase [27–29]; production of charged cluster ions [30]; electron impact ionization of clusters; Coulomb explosion [31,32]; high harmonic generation [33]; photon/electron irradiation [34]; photo-electron spectra of small clusters [35]; nanoplasma generated in atomic and molecular clusters by intense laser pulses [36]; phase diagrams including supercritical phases [37], and eventually, spectroscopy [38] and molecular dynamics studies involving biological media and medical applications [39–42].

The contributions to this issue represent the studies both at the fundamental level of elementary mechanisms

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¹ ICPEAC 2015, <http://www.icpeac2015.com/>

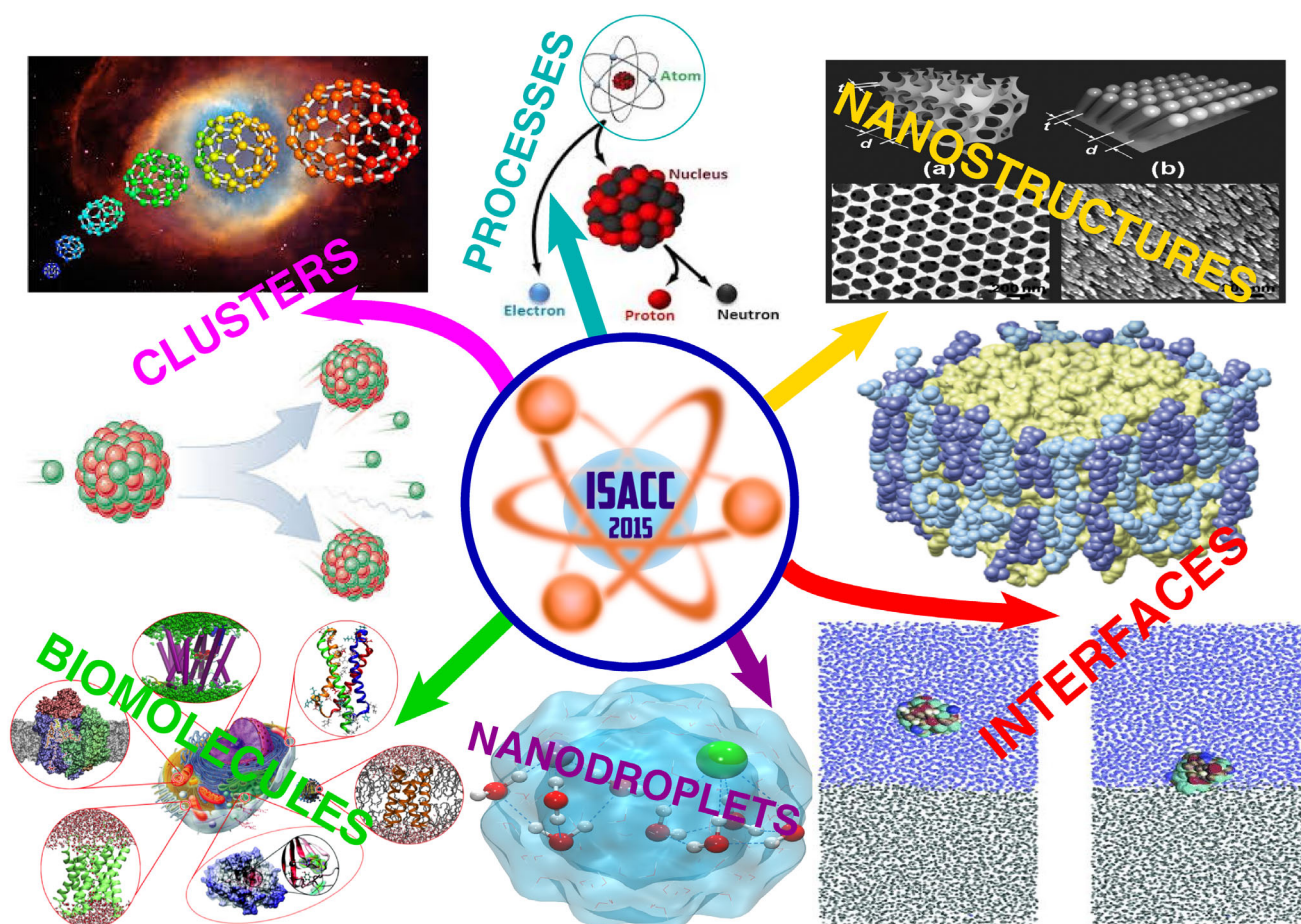


Fig. 1. Topics covered in the ISACC 2015.

and at the more applied level which is necessary in numerous applications of nano- and bio- technology, material science and medicine. Research groups from many countries participate with contributions in this issue and have participated with oral presentations in ISACC 2015. It is noteworthy that among the speakers were several young scientists, who brought new perspectives to their fields.

Following the topics mentioned above, several state-of-the-art methodologies were applied and different processes studied. So, multiconfiguration time-dependent Hartree calculations are presented by Valdés and Prosmiati for the Ar_2ICl vdW cluster characterizing the corresponding states to different isomers [43]. Capture approximations beyond a statistical quantum mechanical method, for atom-diatom reactions, are analyzed by Barrios et al. [44]; for modelling of OH masers, hyperfine resolved collisions of this radical with helium atoms are presented by Marinakis et al. [45]; the reaction of hydroperoxil radicals with ozone, in the presence of water molecules and also inside a water cage of twenty molecules, which is crucial in the atmosphere, is addressed by Viegas and Varandas [46]. Related to chiral molecular recognition phenomena, density functional theory (DFT) is applied by Pelayo et al. to study the

enantiospecific adsorption of cysteine on a chiral Au_{34} cluster [47]. In the framework of nuclear fusion research, calculated electron impact ionization cross-sections of small beryllium-tungsten clusters are reported by Sukuba et al. [48]. Time-dependent DFT coupled to molecular dynamics is employed by Gao et al. to analyze thermal effects on photo-electron emission from small sodium clusters and the C_3 molecule [49]. The effects of quantum confinement on the momentum distribution of electrons confined within a cylindrical potential well are shown by Baltenkov and Msezane [50]. Schütte et al. demonstrate that the formation and decay of doubly-excited atoms and ions is a common phenomenon in nanoplasmas generated by ionization of clusters using intense near-infrared laser pulses [51]. Absolute single carbon loss cross-sections in collisions of helium with native and protonated pyrene cations are measured by Wolf et al. who in addition perform classical Molecular Dynamic simulations to obtain further insight into energy transfer processes [52]. The key role of the spin-orbit interaction onto the properties of sp_2 -carbonaceous fullerenes in the presence of an homogeneous magnetic field is demonstrated by Orlenko et al. [53]; a pseudopotential of C_{60}^- for fullerene-based compounds

is constructed from ab initio quantum-mechanical calculations by Vruble et al. [54]; in the photoionization of noble-gas endofullerenes, as Ar@C₆₀ and Kr@C₆₀, coherence of Auger and inter-Coulombic decay processes are found to govern leading decay mechanisms by Magrakvelidze et al. [55], and in turn, for multishell buckyonions, as C₆₀@C₂₄₀ and C₂₀@C₆₀, photoionization is investigated by means of time-dependent DFT by Verkhovtsev et al. [56]. A molecular dynamics study of accelerated ion-induced shock waves in biological media is presented by de Vera et al. [57]; a novel irradiation driven molecular dynamics approach, which opens a broad range of possibilities for modeling from radiotherapy to focused electron beam deposition, is proposed by Sushko et al. [58], and finally, for medical applications, the coating of gold nanoparticles with polyethylene glycol ligands is studied through classical molecular dynamics by Haume et al. [59].

All in all the 7th ISAAC was very successful meeting, highly appreciated by the attendees. The next ISACC will take place in Varadero (Cuba) on October 2–6, 2017². We expect that future ISACC conferences will be as stimulating as this most recent one was, as indicated by the seventeen high quality contributions of this issue, that can help and motivate future works. We thank all the contributors of this special issue for their participation, the participants, the international and local organizing committees of the ISACC 2015, and the EPJD editorial office for the continuous help and stimulation.

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