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Editorial

Atomic and molecular data and their applications: ICAMDATA 2022

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Abstract. This Editorial provides the general introduction to the collection of papers originated by the 12th ICAMDATA, recalling the inspiring principles of the conference, providing an overview of the advancement in the field of data generation and curation, and illustrating contributions relevant to different applications.

This Topical Issue stems from the 12th International Conference on Atomic and Molecular Data and Their Applications (ICAMDATA), held in Mola di Bari (Italy) in September 2022. The ICAMDATA is a continuing series of international conferences that promotes the use of atomic and molecular (AM) data in various fields of science and technology, fostering cross-disciplinary cooperation between the AM data producers and users, and the coordination of AM data activities and databases worldwide.

The Topical Issue collects 20 papers originating from the contributions presented at the conference. The majority of them are focussed on the theoretical derivation of structural properties of atoms and molecules and of dynamical data (cross sections and rate coefficients) for electron scattering and heavy-particle collision processes, with different approaches. Some papers presenting experimental activity are also included in the collection. Published results contribute to the construction of new knowledge, having an intrinsic and general value, but in many cases aim at giving an answer to specific needs of data in definite fields of application, ranging from astrophysics and fusion plasmas to low-temperature plasmas for technological discharges and aerothermodynamics.

Furthermore, another relevant topic is the data collection and dissemination. The existing infrastructures for data distribution [1–4] are the most valuable tool for the modelling community, and their constant updating process intercepts the ever-increasing level of accuracy and state-selectivity of both computational methods in quantum chemistry and experiments, allowing a scenario of data-from-theory and data-from-experiments. Moreover, they represent the perfect frame for data analysis and the assessment of data quality; this objective intertwined with the need of constructing indicators for the community.

In the following, the contributed papers are briefly introduced to the reader.

The modern techniques in quantum chemistry provide the theoretical framework for the investigation of specific properties of atoms and molecules and of their collisional dynamics that are key in modelling a huge variety of plasma systems, from spectra of kilonovae to magnetically confined tokamak. A selection of cross sections for the electron-impact processes in high-Z atoms (Fe II, Pt III, Au III, W I-II) obtained within the fully relativistic method for atomic structure (GRASP0) and for R-matrix electron scattering (PDARC) by the collision group at Queens University Belfast is presented in Ref. [5].

The pseudo-relativistic Hartree–Fock (HFR) method has been exploited for the investigation on the sensitivity of opacity for uranium (U II and U III) to the inclusion of core polarization effects, still weak, in the calculation of atomic data [6] and also of opacity for lowly and moderately charged lanthanides (Sm V-XI and Nd II-IV) to the inclusion of accurate internal partition functions [7]. These results are relevant to model kilonova spectra and light curves, and in Ref. [8], mathematical inequalities and atomic-physics sum rules are identified as tools for the assessment of the reliability of opacity tables, allowing the derivation of upper/lower bounds.

A special focus is represented by the element tin. In fact, accurate atomic data are expected to impact the analysis of kilonova spectra, but are also relevant to nuclear fusion technology, especially for the design of new-concept plasma facing components in the divertor

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region of the tokamak based on liquid-metal and auto-regenerating plates. In particular, the linearized coupled cluster method in combination with standard ab initio configuration interaction approaches have been used in the derivation of energy levels and multipole forbidden transitions for the singly ionized tin (Sn II) [9], intended for the analysis of the AT2017gfo kilonova emission and for the synthetic spectra generation, while the relativistic convergent close-coupling (RCCC) method has been used to derive a detailed set of electron-impact excitation cross sections for Sn III [10], enlightening the role of inter-channel coupling and the energy limit of validity for approximated approaches.

An intense research activity is devoted to the characterization of highly charged ions in a relativistic framework for the interpretation of the X-ray emission spectra of astrophysical and fusion plasmas. For example, the role of hyperfine-induced multiple interference on the anisotropic character of the angular distribution of the magnetic-quadrupole line of helium-like thallium ions following the electron-impact-induced excitation [11]. Moreover, the process of dielectronic recombination (DR) in boron-like argon [12] and in the helium-like isoelectronic sequence [13] has been investigated based on the relativistic configuration interaction method with inclusion of Breit and QED corrections and the fully relativistic distorted wave approach, respectively. The comparison with measured DR cross sections from high-resolution EBIT (Electron Beam Ion Trap) experiments in modern facilities shows an excellent agreement.

In Ref. [14], the LISA (Lisbon Atomic) database is presented, providing a comprehensive collections of theoretical atomic parameters for X-ray spectroscopy, relevant for example in the characterization of nanomaterials. Data comprise the electron-impact ionization obtained in the modified relativistic binary encounter Bethe model and other structural properties, such as the fluorescence yield of sub-shell or the Coster–Kronig Auger transition yields, derived within ab initio methods in quantum chemistry.

Experiments, on the other hand, can respond to the emerging need of improvements in the accuracy of data and completeness of systems. In this context, the research activity at the Imperial College Spectroscopy group, aiming at the completion of spectroscopic databases, using the Fourier transform (FT) spectroscopy, for the analysis of the astronomical data from ground- and space-based telescopes, is reviewed in Ref. [15], emphasizing the most recent advances.

In Ref. [16], a method is presented for the analysis of complex spectra obtained with the laser-induced fluorescence (LIF) technique (examples are given for the spectra of Zeeman effect for praseodymium and hyperfine structure spectra for niobium) that allows the inclusion of saturation effects in the computer simulations.

Realistic modelling of the plasma edge in fusion devices requires collisional radiative models (CRM) encompassing accurate and complete data for molecular species, principally H_2 and its isotopologues, but also N_2 in the case of nitrogen seeded in the divertor region. The data need are demonstrated in Ref. [17] showing three different levels of detail in the H_2 chemical model in the Yacora solver, i.e. a ro-vibrationally resolved corona model for the Fulcher-α ($d^3\Pi_u \rightarrow a^3\Sigma_g^+$) band, a purely electronic CRM for the singlet electronic terms of the H_2 system, and a vibrationally resolved model for the electronic ground state of H_2. The model implements the most accurate database of electron-impact-induced cross sections obtained with the MCCC (molecular convergent close-coupling) method [18].

The huge number of internal levels to be described, however, is an issue in the kinetic modelling the plasma edge. In Ref. [19], a new model of the collision operator is introduced, i.e. the dressed cross-section model (DCSM), that allows the derivation of an *effective* cross section accounting for multi-step transitions and reducing to the single-step process in the low-density plasma limit, showing the implementation of ionization/recombination into the PIC MC code BIT1 for the simulation of the JET and ITER divertors.

The need of AM data but also of consistency checking and automated data processing is discussed in Ref. [20], presenting the HYDKIN tool with a user-friendly graphical interface, designed to provide input data for the EIRENE Monte Carlo kinetic code for the transport and kinetic simulation in the divertor region of a tokamak.

Low-temperature plasmas are receiving large attention for their potential applications in many fields of technology, and the dynamics of heavy-particle collisions plays a key role in the plasma evolution and in the onset of non-equilibrium conditions in the internal level (vibrational, rotational and electronic) distributions of molecular species. Modelling these plasmas requires the inclusion of the vibrational kinetics and, in turn, the characterization of those processes responsible of the energy transfer between the vibrational/rotational and translational degrees of freedom. The N_2–H_2 inelastic and non-reactive collisions are investigated in Ref. [21] in the framework of the mixed quantum-classical (MQC) method obtaining state-specific rate coefficients for the vibrational energy transfer and also exploring the possibility of exploitation of different machine learning techniques to derive complete datasets.

An interesting approach illustrated in Ref. [22] is intended for the characterization of the stereo-dynamic control of chemi-ionization reactions involving excited metastable noble gas atoms in collisions with an atomic or molecular partner. The reactivity is driven by the optical potential described by using the powerful phenomenological method to derive an accurate an internally consistent formulation of both the real part of the potential, controlling the collision dynamics in the entrance channels, and the imaginary part, determining the probability of the exit channels.

In Ref. [23], the peculiarity in the features of electron scattering cross sections for N_2 and N_2^+ is reviewed, discussing all the processes relevant to nitrogen plasma modelling, offering a critical assessment of the accuracy

of available datasets and including the role of theoretical methods in deriving data for excited states, particularly for the metastable state, still posing difficulties in experiments. This contribution is twinned with an extended paper [24] collecting and creating a database of recommended cross sections for molecular nitrogen.

Another relevant field of application of accurate AM data is the aerothermodynamics, intended for the kinetic modelling of the convective and radiative heat fluxes during the entry phase of space vehicles in planetary atmospheres and for the rationalization of the hypersonic flow experiments carried out in ground-test facilities. In this context, Ref. [25] presents a survey of the experimental radiation data in the vacuum ultraviolet (VUV) region of the spectrum for the creation of a reference database for the future VUV campaign in ESTHER, the European shock tube facility for the preparation of future ESA (European Space Agency) missions.

Finally, in Ref. [26], the analysis performed on the VAMDC (Virtual Atomic and Molecular Data Centre) infrastructure in the framework of the FAIR data maturity model is presented. FAIR principles establish that research data should be findable, accessible, interoperable and reusable, and the paper outlines the principles of FAIRness, illustrating the model indicators as they apply to the VAMDC's services.

The papers presented in this Topical Issue are examples of the intense activity of AM data production, exploiting the capacity of modern theoretical/computational tools in terms of accuracy, specificity and completeness of structural and dynamical data for modelling. Furthermore, the experimental activity is able to respond to the need of data-from-measurements and still fundamental in any validation procedure. Finally, establishing criteria and indicators for the critical and systematical analysis of data in their production, collection and diffusion phases, and formulating new paradigms and best practices (e.g. uncertainty quantification [27]) is a collective process involving the researchers in the community.

We conclude expressing our warmly thanks to all the authors of the papers in this Topical Issue and also the referees for their efforts in reviewing the manuscripts.

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