Recent progress in atomic and molecular physics for controlled fusion and astrophysics

Cite as: Matter Radiat. Extremes 6, 023002 (2021); doi: 10.1063/5.0045218
Submitted: 24 January 2021 • Accepted: 27 January 2021 •
Published Online: 8 March 2021

View Online Export Citation CrossMark

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Note: This paper is part of the Special Issue on Atomic and Molecular Physics for Controlled Fusion and Astrophysics.
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INTRODUCTION

The articles in the "Atomic and molecular physics for controlled fusion and astrophysics" special issue cover a wide range of topics in atomic and molecular physics in the context of hot plasmas. Basic atomic processes are of fundamental importance in confinement fusion and astrophysical environments, and also for ultrahigh–intensity interaction of lasers with matter. Atomic physics in extreme environments such as high pressures and hot or dense plasmas[1,2] presents new challenges to the community, and these have to be addressed by both theoretical and experimental studies. Several extreme configurations are investigated in this special issue, which should be understood as an initiative to draw the attention of the community to important ongoing work in the context of extreme states of matter. This special issue presents eight articles from scientists actively working in this field and shows the important advances that have been made in basic atomic processes and related areas of plasma properties and plasma diagnosis over the last few years.

ADVANCES IN SIMULATING EXTREME PLASMA PROPERTIES

Equation-of-state (EOS) data for deuterium–tritium (DT) mixtures remain of utmost importance for inertial confinement fusion (ICF). Global accurate data for DT covering a wide range of densities and pressures are still lacking and require refinement. Electron–ion interactions present a challenge for first-principles simulations. Kang *et al.*[3] show the importance of electronic many-body effects and nonlocal interactions for obtaining more precise EOS data for DT mixtures under conditions of relevance for ICF. The authors perform *ab initio* simulations over a wide range of parameters, covering densities from 0.1 g/cm^3 to 2000 g/cm^3 and temperatures from about 0.05 eV to 2000 eV. The importance of the ion strong-coupling effect is clearly established, and the results obtained are compared with those from other established methods in the field. Accurate EOS data are important not just for ICF implosions but also for planetary physics and astrophysics.

Modeling of warm dense matter (WDM) properties remains a major challenge. Detailed understanding is of importance, for example, for the study of the interiors of giant planets. At the same time, it is also crucial for ICF. Dynamic compression of matter with X-ray pulses produces short-lived, spatially inhomogeneous states. Detailed knowledge of such nonequilibrium (transient) WDM states is important. Kang *et al.*[4] investigate hydrogen WDM using a two-temperature approach, i.e., considering conditions where the electron temperature T_e and ion temperature T_i are not equilibrated. Investigating warm dense hydrogen in a two-temperature situation is challenging owing to nuclear quantum effects (NQEs), which affect the structure and thermodynamic properties and thereby reveal the limitations of ordinary *ab initio* molecular dynamics. The authors perform orbital-free-driven path integral PIMD (PI-OFMD) simulations and systematically estimate nuclear quantum effects.

NEW TOOLS FOR PLASMA DIAGNOSTICS

With several multi-petawatt laser installations coming online worldwide, an urgent issue is reliable characterization of the focused intensity of such laser pulses. For experimental purposes, it is important to know the *in situ* laser intensity while minimizing the impact of the environment on the focal spot itself. Ciappina *et al.*[5] investigate the possibility of characterizing ultrahigh laser intensities in the focal spot by analyzing ionization states of high-Z elements in a low-density gas. They show that the geometry of the focal spot can be analyzed through the signatures of the tunnel ionization yields, providing detailed information about the intensity distribution. They present several algorithms for extracting the relevant information from potential time-of-flight measurements and compare them. *In situ* information about electromagnetic field strengths provides an extremely valuable boundary condition for laser–matter interaction experiments.

X-ray spectroscopy is an extremely valuable tool for investigating hot inertial thermonuclear plasmas. For it to be applicable, the spectroscopic parameters of multicharged ions need to be known, in particular the wavelengths of radiative transitions. As atomic models of high-Z multicharged ions are extremely complex, experimental validations are required. In general, the predicted wavelengths of resonance transitions in He- and Li-like ions are crosschecked against precise spectroscopic measurements that use the spectral lines of H-like ions for spectral calibration. However, for high-Z elements, it is difficult to create a hot dense plasma with a large concentration of H-like charge states. In the article by Ryazantsev *et al.*,[6] mineral-based laser targets comprising elements with moderate (between 15 and 30) and low (less than 15) Z are investigated, with emission from the latter delivering perfect reference lines over a whole range of He- and Li-like moderate-Z emission under examination.

Wang and Zhu[7] provide a detailed overview of recently developed experimental methods for nonresonant inelastic X-ray scattering (NRIXS). NRIXS enables determination of the electronic structure and dynamic parameters of atoms and molecules in momentum space. This method allows evaluation of the form factors, oscillator strengths, and Compton profiles of atoms and molecules. New insight into excitation mechanisms can be obtained. A comparison with other methods is presented, and the potential of NRIXS for future applications in atomic and molecular physics is described.

THE CONTINUED IMPORTANCE OF BASIC ATOMIC PROCESSES

Many plasmas that are encountered are in a state that is not in local thermodynamic equilibrium (LTE) and are therefore challenging from the atomic physics point of view. In the article by Rosmej *et al.*,[8] novel phenomena and methods related to dielectronic recombination in such non-LTE plasmas are investigated, and the importance of excited states in this respect is shown. The authors derive simple analytical formulas to study these processes. They show that standard approaches overestimate the total dielectronic recombination rates by several orders of magnitude. It is explained that this originates from the suppression of higher-order contributions due to multichannel auto-ionization and radiative decay. Accurate knowledge of correct atomic populations is relevant, for example, to EOS data and radiative properties of matter, directly influencing fusion science, planetary properties, and astrophysical phenomena.

In astrophysical plasmas, photoionization is one of the most important processes that occur. It also plays a fundamental role in indirect drive configurations in ICF for ionizing the inner wall of the hohlraum. Laser-driven light sources such as high-harmonic generation and free-electron lasers are driving interest in the photoionization of inner atomic and ionic shells. Reliable cross-sectional data for photoionization of complex atoms are required in order to enable high-quality predictive simulations in light–matter interaction. Rosmej *et al.*[9] present new generalized methods that are suitable for integrated simulations of the photoionization process. They employ statistical methods with the local plasma frequency approach to study the photoionization cross-sections of complex atoms.

Gao *et al.*[10] investigate theoretically the details of the processes of projectile and target excitation occurring in He^+ + He collisions. They point out the importance of highly excited states in the basis set used in calculations for agreement between theory and experiment. They also establish the importance of nonperturbative calculations in which a sufficient number of channels are taken into account. In the collision energy range from 3 keV/amu to 225 keV/amu, very good agreement with available experimental data is obtained. New insights into electronic excitation processes are provided.

The atomic physics occurring in high-energy-density situations will be complex, because many simultaneous atomic processes are present, mutually affecting each other. The articles in this special issue recognize some aspects of this problem. However, well-planned and thoroughly analyzed experiments are required to test the theory and simulations developed.

The famous Macedonian atomic physicist Professor Ratko Janev (March 30, 1939–December 31, 2019) had worked with us to start commissioning this special issue, and he promised to contribute an article to it. We are very sorry to hear that he passed away from illness. We have lost an important physicist and dear friend. The scientific community has lost a leading scientist in the field and will miss him a lot. Professor Janev was a member of the Macedonian Academy of Sciences and Arts. He was a prominent scientist for more than 30 years from 1986 onward, and he contributed extensively to the international atomic and molecular physics community, especially in the context of hot plasmas. He published more than 300 scientific papers, including one in MRE in 2016.[11] Professor Janev will live in our memory, and we will carry on his scientific legacy.

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