PHYSICAL AND TECHNOLOGICAL SCIENCES

Atomic Theory Group

Vilnius University

Keywords: *atomic, molecular and solid-state parameters, electron-ion and photon-ion interaction, plasma.*

Research group activities

The aim of our activities is to provide atomic, molecular, and solid-state data needed for various industrial areas, especially high-tech (including space and military industry) sectors. These data are crucial for modeling the radiative properties of ions and atoms in plasmas ranging from the interstellar medium to the solar atmosphere and experimental thermonuclear devices. Within this field, our work covers studies of spectroscopic properties and interaction of electrons and photons with atoms leading to emission spectra modeling.

Main area of interest is modeling of processes in plasmas related to production of carbon-free energy in fusion power plants. Many properties of fusion plasma are determined by radiation from impurities. Energy loss from heavy elements, such as tungsten, due to radiative emission is one of the crucial obstacles to be overcome for the successful performance of thermonuclear reactors. The ionization and recombination processes determine the charge-state distribution in plasma. Thus, one of our research activities is devoted to the study of direct and indirect ionization processes.

A significant focus of our research has been on the solid-state field, the microscopic and macroscopic elastic parameters of perovskite crystals obtained from first-principles calculations. These characteristics are necessary for the effective fabrication of thin-film devices with broad functionalities.

Many of the problems humans currently face can be solved by developing new materials. Thus, the results of theoretical modeling and research of new molecules and their derivatives are likely to affect significantly the future of technology.

Proposal

We offer our experience and such services as:

- Atomic and molecular data production;
- Spectroscopic parameters database;
- Plasma spectra modeling;
- Computer programming;
- Solid-state modeling;
- Modeling and investigation of molecules and their derivatives.

We seek partners for collaboration within atomic, molecular and solid-state area of research.

We seek partners for developing competitive research projects targeting HORIZON 2020 and other international programs.

Meet our team

Head - Dr. Valdas Jonauskas

Research staff - Dr. Gediminas Gaigalas, Dr. Romualdas Karazija, Dr. Alicija Kupliauskienė, Dr. Rasa Karpuškienė, Dr. Romualdas Kisielius, Dr. Sigitas Kučas, Dr. Jelena Tamulienė, Dr. Rytis Juršėnas, Dr. Aušra Kynienė, Dr. Šarūnas Masys, Dr. Alina Momkauskaitė, Dr. Laima Radžiūtė, Dr. Pavel Rynkun

PhD students - Gintaras Kerevičius, Jurgita Koncevičiūtė, Saulius Pakalka

Research outcomes

Methods and computer codes developed to deal with correlation effects and angular integration in atomic structure calculations, which enable us to produce highly accurate atomic data. Online database ADAMANT (www.tfai.vu.lt/database) for plasma spectra modeling.

Selected publications:

- **A. Kynienė, Š. Masys, and V. Jonauskas,** Influence of excitations to high-nl shells for the ionization process in the W26+ ion, Phys. Rev. A 91, 062707 (2015).
- **L. Radžiūtė G. Gaigalas, P. Jönsson, J. Bieroń,** Electric dipole moments of superheavy elements: A case study on copernicium, Phys. Rev. A 93, 062508 (2016).
- **S. Grebinskij, Š. Masys, S. Mickevičius, V. Lisauskas, V. Jonauskas.** Ab initio and photoemission study of correlation effects in SrRuO3 thin films, Phys. Rev. B 87, 035106 (2013).
- **J. Tamuliene, J. Noll, P. Frenzel, T. Rüffer, A. Jakob, B. Walfort, H. Lang,** Synthesis of [{AgO 2 CCH 2 OMe(PPh 3)} n] and theoretical study of its use in focused electron beam induced deposition, Beilstein J. Nanotechnol. 8, 2615-2624 (2017).
- **F.H. Cashman, V.P. Kulkarni, R. Kisielius, G.J. Ferland, P. Bogdanovich.** Atomic Data Revisions for Transitions Relevant to Observations of Interstellar, Circumgalactic, and Intergalactic Matter, The Astrophysical Journal Supplement Series, 230, 8 (2017).

Collaboration with:

- National Institute of Standards and Technology, USA - identifying spectral lines obtained from experimental measurements;
- National Institute for Fusion Science, Japan - analysing spectroscopic properties of Er2O3 crystal used for inner wall in fusion plants. Produced data helped our partners to model damage level of the material;
- Department of Physics and Astronomy, University of South Carolina, Columbia, USA – atomic data used to evaluate a chemical evolution of Universe;
- Materials Science and Electrical Engineering Department at the Center for Physical Sciences and Technology, Lithuania;
- Vilnius University, Life Sciences Center, Lithuania.

Contacts

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