Study of electron-iodine molecule collisions for electric space propulsion.

Synopsis

The aim of the PhD project is to investigate theoretically electron collisions with iodine compounds. The corresponding cross sections will be computed using an R-matrix approach which includes for the first-time spin-orbit coupling effects. The latter are expected to have a significant impact for molecules containing iodine. The results of this project will be used for plasma simulations and electric propulsion applications. The PhD will be done in co-tutelle with Dr Zdeněk Mašín from Charles University. The PhD student will also benefit from the collaboration with Dr Anne Bourdon, from Laboratoire Physique des Plasma, for the plasma simulations. An industrial partner, Quantemol Ltd (a UK-based company), will advise on potential applications of the calculated data for the development of commercial propulsion devices.

Introduction, scientific context and objectives

Electron-scattering cross-section data for iodine compounds are important for plasma simulations and electric propulsion applications. Indeed, recent developments in iodine-based electric thrusters[1] [1-2] resulted in an increasing need for electron collision cross sections. For example, in Hall-effect thrusters electrons emitted from the cathode interact with the gas from the anode. Therefore, studies of electron-driven processes are crucial to improve the modeling of iodine plasma and thus to advance the performance of iodine-based electric propulsion thrusters.

Electron collisions with I and I_2 have been recently investigated in [3] by Quantemol Ltd. However, spin-orbit coupling effects were neglected in this work. The latter effects are expected to be significant in iodine compounds. Accurate calculations of electron-scattering cross sections should therefore take relativistic effects into account. The aim of this PhD project is to implement the spin-orbit coupling effects in the UK-Rmol+ package [4]. The latter is an efficient implementation of the R-matrix electron-molecule scattering approach. With this new code, the PhD student will investigate the processes taking place in electron-iodine molecule collisions.

To achieve the goals of the PhD project, the student will be co-supervised by the principal investigator at Sorbonne Université (N. Sisourat) and by Dr Zdeněk Mašín from Charles University. Dr Zdeněk Mašín is the main developer of the UKRmol+ package and he is an expert in electron-scattering processes. It should be noted that Sorbonne Université and Charles University are major partners in the 4EU+ Alliance. The proposed project will initiate a new collaboration between the two groups and therefore strengthen the links between the two universities. Furthermore, the PhD student will benefit from the undergoing collaboration with Dr Anne Bourdon, from Laboratoire Physique des Plasma. Dr Anne Bourdon has a recognized expertise in plasma simulations and especially in iodine plasma. Quantemol Ltd. has a long history, since 2004, as the provider of electron scattering data for industrial applications. The company will guide us and the student on the type and format of data needed for practical applications. The company is prepared to step in with a financial contribution in case an opportunity to commercialize the results of the research appears. The complementary expertise of our research groups and the connection with industry is a major asset of the project.

Research methodology and PhD project

The relativistic effects to be included in the project can be represented accurately within the framework of first order perturbation theory [5] with the Pauli Hamiltonian. This approach will be a simplified, yet sufficiently accurate, version of an existing semi-relativistic atomic R-matrix approach [6]. The Pauli Hamiltonian contains only one-body operators which describe relativistic effects up to order $O(c^{-2})$. Inclusion of those effects will require implementation of matrix elements of those operators. The evaluation of the spin-orbit integrals will follow the method of Kuang [7]. Currently, an alternative approach based on effective core (relativistic) potentials is under development by Dr Mašín and the student will have the opportunity to compare both approaches to study the relativistic effects at a deeper level.

We will implement the relativistic coupling matrix elements of the Pauli approach into the UKRmol+ package. This task will be done by Dr Zdeněk Mašín and the PhD student. Using this code, the PhD student will compute the electron impact excitation cross sections for iodine molecule and its ions. The implementation of the relativistic terms in the the UK-Rmol+ code is expected to take one year. The second and third years will be devoted to the study of electron-driven processes in iodine plasma. The fourth (wrap-up) year will be covered by the partner at Charles University. The results will shed light on the relativistic effects on electron-scattering data,

[1] 1/ The first launch of a satellite using iodine plasma took place recently (on November 6, 2020) with a thruster developed by the French start-up ThrustMe on a satellite of the Chinese aerospace company SpaceTy.

as well as provide accurate cross sections for plasma modelling and electric propulsion applications.

Nicolas Sisourat will advise the PhD candidate on the *ab initio* study of electron-scattering processes. He has over 10 years of experience in the simulation of inelastic electronic processes and has developed several state-of-the-art codes for such simulations. Zdeněk Mašín is the main developer of the UKRmol+ package and he is an expert in electron-scattering processes. He will co-advise the PhD student and help in the implementation of the relativistic terms in the UKRmol+ code. Anne Bourdon is an expert in plasma modelling and will be a complementary help for the PhD candidate on the electric propulsion applications.

Originality and innovative aspects of the proposal

Molecular propellants for electric thrusters are currently investigated worldwide. Iodine molecule is a promising candidate since it has a high atomic mass and low ionization potential, which are essential for efficient propulsion. Furthermore, iodine is cheap and exists in the solid state at standard pressure and temperature. The latter property results in a high storage density of propellant. However, iodine molecule is highly electronegative and thus has a rich chemistry which is not well understood yet.

The proposed PhD project will significantly contribute to fill this gap. To achieve the scientific goals a trans-disciplinary approach is essential. We will tackle the challenging task of treating electron-iodine collisions with a relativistic description, going beyond the current state of the art. The results will be used for iodine plasma modelling. The project will therefore have a significant impact in the rapidly growing field of electric propulsion.

Relevance of the project for the Initiative Physique des infinis

As detailed above, the aim of the PhD project is to provide an accurate description of electron-driven processes in iodine plasma thrusters. Such a fundamental and ambitious goal requires a greatly improved understanding of the atomic and molecular processes in plasma. Furthermore, the demand for small electric-powered satellites is rising quickly due to their commercial and military applications. This PhD project will therefore have a significant societal impact. These objectives are at the core of the Initiative Physique des infinis.

References

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Profile of the PhD Applicant

The PhD applicant should have a master's degree in chemistry or physics. She/He should have good competence in programming and numerical methods. Knowledge in plasma physics and/or theoretical chemistry approaches will be an asset.