SORBONNE UNIVERSITÉ

**PROGRAMME INSTITUTS ET INITIATIVES**

**Appel à projet – campagne 2021**

**Proposition de projet de recherche doctoral (PRD)**

# IPhyInf - Initiative Physique des infinis

**Intitulé du projet de recherche doctoral (PRD):**

## Recombination reactions at the walls of iodine plasma

**Directeur de thèse porteur du projet (titulaire d'une HDR) :**


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**Unité de Recherche :**
Intitulé : Laboratoire Chimie Physique Matière et Rayonnement
Code: UMR 7614


**École Doctorale de rattachement de l'équipe (future école doctorale du.de la doctorant.e) :** ED388-ChimiePhysique&ChimieAnalytique ParisCentre

**Doctorant.e.s actuellement encadré.e.s par la.e directeur.rice de thèse: 0**

**Co-encadrante :**


NOM : **BOURDON** Prénom : **Anne**
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**Unité de Recherche :**
Intitulé : Laboratoire de Physique des Plasmas (LPP)
Code: UMR 7648


**École Doctorale de rattachement :** Choisissez un élément :
Ou si ED non Alliance SU : **École doctorale de l'Institut Polytechnique de Paris (ED IP Paris)**

**Doctorant.e.s actuellement encadré.e.s par la.e co-directeur.rice de thèse : 1 (1ère année de thèse , 33%) 3 (2ème année de thèse, 33%)**

**Cotutelle internationale :** ☒ Non ☐ Oui, précisez Pays et Université :

**Selon vous, ce projet est-il susceptible d'intéresser une autre Initiative ou un autre Institut ?**
☒ Non ☐ Oui, précisez Choisissez l'institut ou l'initiative :

**Description du projet de recherche doctoral *:***

**Introduction, scientific context and objectives**

Iodine is currently under investigation as an alternative propellant in electric thrusters for space vehicles [1]. However, there are many technical challenges in designing electric thrusters that use iodine, including the fact that it can condense and can corrode satellite materials [2]. Therefore, the first launch of a satellite using iodine plasma took place only very recently (on November 6, 2020) with a thruster developed by the French start-up ThrustMe on a satellite of the Chinese aerospace company SpaceTy.
Up to now, only the mechanical and thermal issues with iodine use were addressed. **The next step for the development of efficient iodine plasma based thrusters is to improve the control of the iodine plasma itself.** In such thrusters, electrical energy is supplied to the electrons to ionize the iodine molecules and thus to form a plasma. However, due to the molecular nature of this gas, electron energy is inevitably dissipated in other processes including dissociation as well as electronic, vibrational and rotational excitation. These processes produce various atomic and molecular iodine species, both neutral and ionized. Only ions can be electrically accelerated to produce thrust. However, ions are lost through various reactions (recombination, neutralisation) both in the volume of the plasma and at the reactor surfaces, causing substantial power loss. There is currently little reliable data available on most of these processes, preventing a valid description and modeling of iodine plasmas for electric propulsion.
The aim of this PhD project is to obtain accurate rates of the loss processes of the variuous transient species at the reactor surfaces. **To achieve this goal, we will combine high-level *ab initio* calculations (done at LCPMR) with plasma models of a prototype thruster studied at LPP.** The complementary expertise of our groups is a major asset of the project.

**Research methodology and PhD project**

The major loss reaction of atomic iodine is the recombination of the atoms into iodine molecules at the reactor surfaces. At LPP, an experimental work is underway to better characterize an iodine plasma in a simplified geometry thruster (based on the thruster PEGASES patented in 2007 at LPP). Preliminary experiments have shown the feasability of the measurements of recombination rates at the reactor surfaces [3]. Iodine atoms will be detected by diode-laser absorption spectroscopy, using the 1315nm spin-orbit transition [4]. Measurements using a dual-beam absorption technique in pulse-modulated plasmas will provide the surface recombination probability from the atom lifetime in the afterglow. The

objective of the proposed PhD project is to develop models to compare with these measurements.
First we will simulate from first principles the recombination processes at the reactor surfaces and compute their reaction rates. We will employ high-level *ab initio* electronic structure calculations and advanced molecular dynamics simulations [5]. The reaction rates will be obtained using a semiclassical approach in which the dynamics of the recombining atoms follow classical trajectories while the electronic interactions between them and with the reactor walls are treated quantum mechanically. The aluminium walls of the PEGASES reactor will be modeled using Density Functional Theory (DFT) as implemented in VASP [6]. The theoretical recombination rates will be compared to the measured ones.
The PhD student will then implement the rates of the recombination on the walls in an existing fluid model of the iodine plasma. The model and corresponding codes are developed at LPP. The results of this fluid model can be compared with the plasma measurements on PEGASES. Note that the PhD student will assist to a few measurement campaigns to better understand the experiments and the corresponding results. The complementary of the groups and comparing theoretical results with experiments made at LPP is a strong asset of the PhD project.

Nicolas Sisourat will advise the PhD candidate on the *ab initio* study. 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. Anne Bourdon is an expert in plasma modeling, and will be the advisor of the PhD candidate for the electric propulsion applications.

## Originality and innovative aspects of the proposal

Although iodine was first proposed as an alternative propellant nearly 20 years ago [7,8], there have been only a few experimental investigations of their performance (see [9,10] and references therein). **Furthermore, to our knowledge, there have been only two modeling studies of the iodine plasma composition [11,12] due to the lack of available data.**
This 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 considering different aspects of an iodine plasma. Combination of high-level electronic structure calculations, simulations of atomic and molecular collisions and plasma models, compared to specifically designed experiments, will enable description of iodine plasmas with vastly improved accuracy. **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 pave the way to an accurate description of iodine plasma thrusters. Such a fundamental and ambitious goal requires a greatly improved understanding of the atomic and molecular processes taking place at the walls of the plasma reactors. Furthermore, the demand for small electric-powered satellites is rising quickly due to their commercial and military applications [13-15]. This PhD project will therefore have a significant societal impact. These objectives are at the core of the Initiative Physique des infinis.
It should be mentioned that we have been awarded for a 12 months postdoctoral grant last year (IPhysInf-AAP2020-Postdoc; recruitment of the postdoctoral researcher is underway but due to the COVID pandemic finding a suitable candidate is difficult). This proposed PhD project is complementary to the postdoctoral project: the PhD student will investigate the reactions at the walls of iodine plasma reactors while the postdoctoral researcher will focus on the

neutralisation reactions taking place in the volume of these plasma. However, a strong interaction between the PhD student and the postdoctoral researcher is expected, which will be beneficial to both of them.

**References**


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[2] H. Kamhawi et al. 52nd AIAA/SAE/ASEE Joint Propulsion Conference (2016); P. Dietz et al. Eur. Phys. J. Appl. Phys. **91**, 10901 (2020).
[3] F. Marmuse et al. Proceedings of the IEPC conference (2019).
[4] Ha et al. Phys. Chem. **99**, 384 (1995).
[5] M. Cacciatore and M. Rutigliano Int. J. Quantum Chem. **106,** 631 (2006) and references therein.
[6] G. Kresse and J. Hafner, Phys. Rev. B **47** , 558 (1993); ibid. **49** , 14 251 (1994).
[7] R. Dressler, Y.-H. Chiu, and D. Levandier, 38th Aerospace Sciences Meeting and Exhibit (2000).
[8] O. Tverdokhlebov and A. Semenkin, 37th Joint Propulsion Conference and Exhibit (2001).
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[10] T.D. Smith et al. NASA Technical reports (2016).
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**Publications of the advisors that are relevant for the present proposal**


1) B. Casier, S. Carniato, T. Miteva, N. Capron and N. Sisourat, J. Chem. Phys. **152**, 234103 (2020).

2) S. Kazandjian, J. Rist, M. Weller, F. Wiegandt, D. Aslitürk, S. Grundmann, M. Kircher, G. Nalin, D. Pitters, I. Vela Pérez, M. Waitz, G. Schiwietz, B. Griffin, J. B. Williams, R. Dörner, M. Schöffler, T. Miteva, F. Trinter, T. Jahnke and N. Sisourat, Phys. Rev. A. Rapid. Comm. **98**, 050701 (2018)

3) V. Croes, A. Tavant, R. Lucken, R. Martorelli, T. Lafleur, A. Bourdon and P. Chabert, Physics of Plasmas **25**, 063522 (2018).

4) P. Grondein, T. Lafleur, P. Chabert, and A. Aanesland, Physics of Plasmas **23**, 033514 (2016).


**Profile of the PhD Applicant**

The PhD applicant should have a master 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.