# Plasma Surface Interaction (Data and Tools) COupled Modelling (PSI.COM)

## WE ARE HIRING - Call for Expressions of Interest

Project PSI.COM addresses the coupled modelling of the plasma-surface chemistry in $N_2$-$H_2$ mixtures, comprising several exciting endeavours: bridging the gap between volume and surface reactivity in plasma simulations; exploring the full potential of high-quality controlled measurements in an interplay with self-consistent time-dependent kinetic simulations; embracing screening/reduction of chemistry schemes as key-component of modelling; and publishing validated data in web-based platforms.

We will leverage on complementary expertise in modelling and diagnostics of low-temperature plasmas (LTP) from group N-PRiME (N-Plasmas Reactive: Modelling and Engineering, Instituto de Plasmas e Fusão Nuclear – IPFN, Instituto Superior Técnico – IST, Lisbon Portugal) and from LPP (Laboratoire de Physique des Plasmas, Ecole Polytechnique, Palaiseau, France).

Project tasks involve

(i) the study of N2-H2 plasmas and the catalytic production of ammonia, using an interplay between modelling and diagnostics to understand the volume + surface kinetic paths, and to validate and reduce the kinetic scheme;

(ii) the development and the consolidation of the LoKI tool suite, aiming at full time-dependent description, extended to surface reactions and including the gas/plasma thermal balance, and including ML tools for sensitivity analysis;

(iii) the formulation and implementation of solutions for data storage and parsing in LTPs modelling, aiming at developing a high-performance open-access data-storage library for LoKI, in association with the LXCat stakeholders.

**PSI.COM is currently inviting expressions of interest (EoI) for**

- **a three-year postdoctoral position at IPFN/IST, mainly to develop tasks (i) and (ii), starting on mid-March 2023** (here, we prefer candidates with previous experience in the modelling of low-temperature plasmas)

- **a two-year contract with an institution affiliated to IST, mainly to develop tasks (ii) and (iii), starting early 2024** (here, we prefer candidates with technical skills in the development of scientific software and of platforms for data storage, analysis, and visualization.

**For more information, please contact Prof. Luís L. Alves at** llalves@tecnico.ulisboa.pt
(message subject: "PSI.COM"; for an expression of interest please join your CV)
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