

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

WE ARE HIRING A RESEARCH ENGINEER - 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 N_2 - H_2 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 LisbOn Kinetics (LoKI) tool suite** (<https://nprime.tecnico.ulisboa.pt/loki/>), aiming at full (Boltzmann+Chemistry) time-dependent description, extended to surface reactions and including Machine Learning tools for sensitivity analysis;
- (iii) the contribution to the **development of a high-performance open-access data-storage library for LoKI**, in association with the LXCat stakeholders (<https://lxcat.net>)

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

- a **two-year Research Engineer contract (gross salary ~1.3k€), starting in the spring of 2024, with focus on task (iii)** (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)