

PiAI Seminar Series: Physics informed AI in Plasma Science

10:00-11:00, 03 June 2024 (CEST)

9:00-10:00, 03 June 2024 (WEST)

17:00-18:00, 03 June 2024 (JST)

Web Seminar

Deep Learning for Plasma Chemistry Modelling

Matilde Valente, Marcelo Gonçalves, Tiago Dias, Rodrigo Ventura, Vasco Guerra

Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal

Low-temperature plasmas (LTPs) are versatile in their applications, finding uses in areas ranging from plasma medicine to CO₂ conversion for *in-situ* resource utilisation. Understanding these systems requires a combination of experimental data and the development of predictive plasma-chemistry models. However, obtaining experimental data is challenging, and plasma simulations are often computationally expensive. Here, we explore deep learning to mitigate these difficulties with a twofold approach: on the one hand, we create a fast and reliable surrogate model to study the complex plasma chemistry in low-pressure molecular plasmas; on the other hand, we automate the prediction of selected reaction rate coefficients. Moreover, we propose a novel approach for integrating physical constraints into deep neural networks by projecting the model's predictions onto the manifold defined by the system's physical constraints. Oxygen DC discharges at pressures $p = 0.2 - 10$ Torr and discharge currents $I = 10 - 40$ mA are used as a case study.