

Proposal of research subjects for training

group N-Plasmas Reactive: Modelling and Engineering (N-PRiME)
Instituto de Plasmas e Fusão Nuclear (IPFN)

<https://www.ipfn.tecnico.ulisboa.pt/nprime/opportunities.html>



**In case of interest, please email directly
the contact person in each proposal**

2024

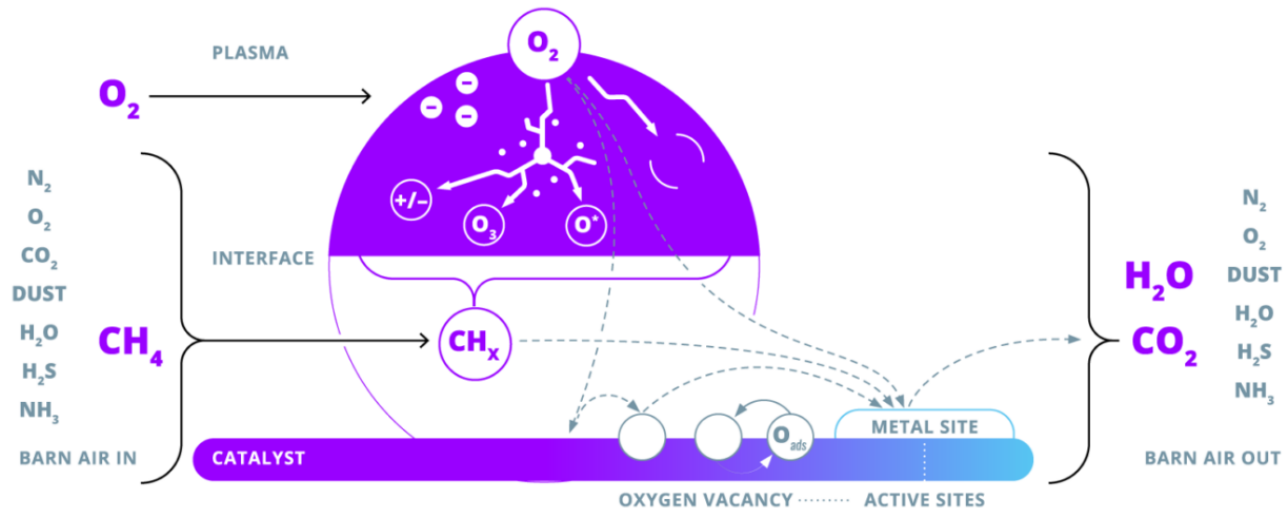
Title: Microscopic simulations of plasma-catalysis interactions for methane abatement

Supervisors: Pedro Viegas (pedro.a.viegas@tecnico.ulisboa.pt), IPFN/IST-UL, Karina Shimizu (karina.shimizu@tecnico.ulisboa.pt), CQE/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Abstract

A sustainable economy requires the recycling of greenhouse gases into useful products (e.g. CH_4 and CO_2 into CO , H_2 and O_2). In particular, the farming sector needs to reduce methane emissions by oxidizing that gas. For this conversion process, low-temperature plasmas are essential, in interaction with solid-state catalysts, electrolyzers and other surfaces. Low-temperature plasmas are electrically-powered reactive gases with ideal conditions for gaseous conversion, while solid-state materials can promote specific reactions and be highly selective to certain species. To merge the two technologies is a novel approach with increasing attention, but the interaction between plasma species and surface materials is still mainly unknown.

In this project, a software package will be used to perform Density Functional Theory calculations, based on the quantum mechanical description of the electronic structure of many-body systems. These will focus on specific reactions of interest of plasma-catalysis systems for gaseous conversion, which have never been studied. The project will be supervised by DFT experts and plasma researchers together, within the cadre of the CANMILK European project (canmilk.eu) developing technologies for greener milk production. International collaborations are in place and research stays are possible at partner institutions in Belgium, The Netherlands or The United Kingdom, among others.



Goals

In this project, a software package will be used to perform Density Functional Theory calculations, based on the quantum mechanical description of the electronic structure of many-body systems. These will focus on specific reactions of interest of plasma-surface systems for methane oxidation and gaseous conversion, which have never been studied.

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, internship

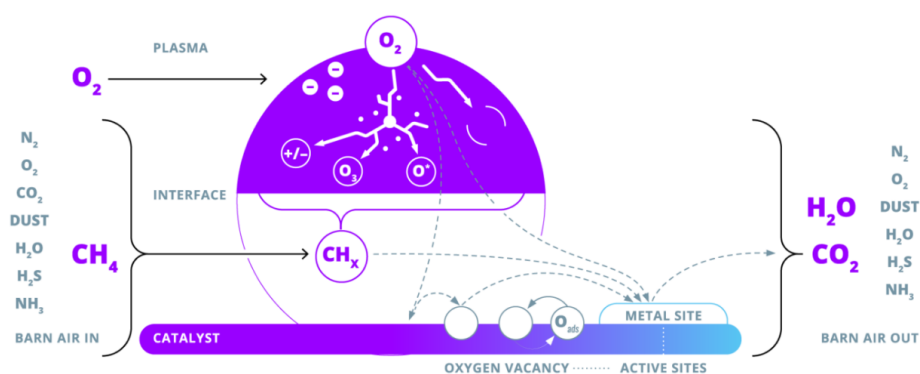
Title: Modelling plasma-surface interactions in plasmas for CH₄ oxidation

Supervisors: Pedro Viegas (pedro.a.viegas@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Abstract

A sustainable economy requires the recycling of greenhouse gases into useful products (e.g. CH₄ and CO₂ into CO, H₂ and O₂). In particular, the farming sector needs to reduce methane emissions by oxidizing that gas. For this conversion process, low-temperature plasmas are essential, in interaction with solid-state catalysts, electrolyzers and other surfaces. Low-temperature plasmas are electrically-powered reactive gases with ideal conditions for gaseous conversion, while solid-state materials can promote specific reactions and be highly selective to certain species. To merge the two technologies is a novel approach with increasing attention, but the interaction between plasma species and surface materials is still mainly unknown.

In order to understand, predict and optimize plasma-catalysis reactor performance for CH₄ abatement, it is essential to describe plasma-surface interactions. The aim of this work is to develop the numerical framework to describe the formation of molecules as a result of the interaction between the reactive species created in a plasma, adsorbed barn methane and catalyst surfaces. The model development will start from existing models of the research team that separately describe the plasma production and maintenance and surface processes in different systems. The surface kinetics model will account for the elementary steps of physisorption, thermal desorption, chemisorption, and both Eley-Rideal and Langmuir-Hinshelwood recombination of adsorbed species. The simulations will be carried out with numerical codes available for oxygen or CO₂, that shall be modified to account for new elementary processes. The project will be supervised by plasma researchers in close contact with surface experts, within the cadre of the CANMILK European project (canmilk.eu) developing technologies for greener milk production. International collaborations are in place and research stays are possible at partner institutions in Belgium, The Netherlands or The United Kingdom, among others.



Goals

The aim of this work is to develop the numerical framework to describe the formation of molecules as a result of the interaction between the reactive species created in a plasma, adsorbed barn methane and catalyst surfaces.

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, internship

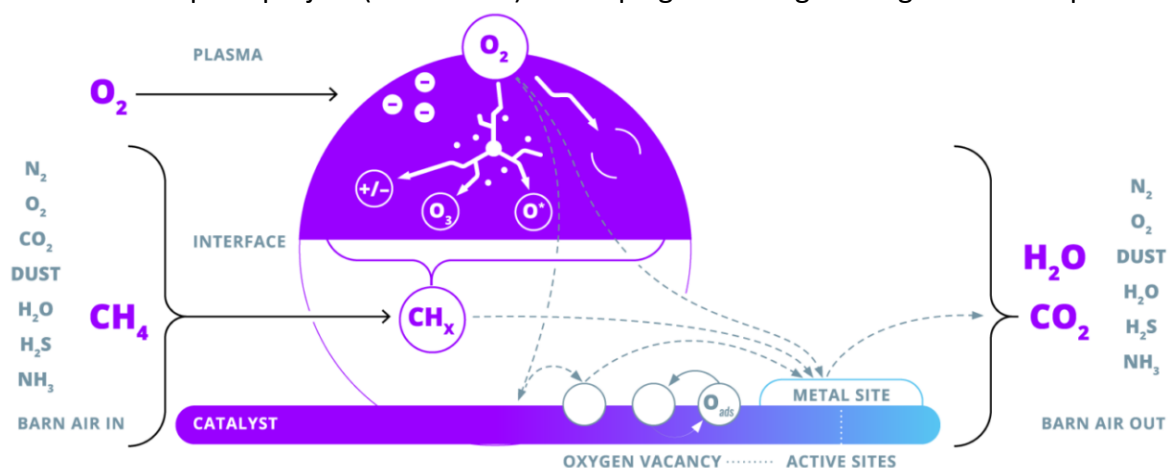
Title: Experimental measurement of CH₄ oxidation via plasma-catalysis synergies

Supervisors: Pedro Viegas (pedro.a.viegas@tecnico.ulisboa.pt), IPFN/IST-UL, Carmen Bacariza (mari.rey@tecnico.ulisboa.pt), CQE/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Abstract

A sustainable economy requires the recycling of greenhouse gases into useful products (e.g. CH₄ and CO₂ into CO, H₂ and O₂). In particular, the farming sector needs to reduce methane emissions by oxidizing that gas. For this conversion process, low-temperature plasmas are essential, in interaction with solid-state catalysts, electrolyzers and other surfaces. Low-temperature plasmas are electrically-powered reactive gases with ideal conditions for gaseous conversion, while solid-state materials can promote specific reactions and be highly selective to certain species. To merge the two technologies is a novel approach with increasing attention, but the interaction between plasma species and surface materials is still mainly unknown.

In order to understand, predict and optimize plasma-catalysis reactor performance for CH₄ abatement, it is essential to describe plasma-surface interactions. The aim of this work is to experimentally quantify the formation of molecules as a result of the interaction between the reactive species created in a plasma, adsorbed barn methane and catalyst surfaces. The experiments will take place in world-class laboratories abroad, fully equipped for plasma-catalysis set-ups and Fourier Transform Infra Red (FTIR) measurements. Such measurements will improve our understanding of catalytic surface reactivity in the presence of plasma, inclusively by allowing the validation of plasma-surface kinetics models. The project will be supervised by experimental plasma and catalysis researchers in close contact with modelers in Portugal, within the cadre of the CANMILK European project (canmilk.eu) developing technologies for greener milk production.



Goals

The aim of this work is to experimentally quantify the formation of molecules as a result of the interaction between the reactive species created in a plasma, adsorbed barn methane and catalyst surfaces.

Period: School year 2024/2025

Framework: PIC2/MSc thesis, internship

Title: Multidimensional fluid modelling of plasma-membrane systems for gas conversion

Supervisors: Pedro Viegas (pedro.a.viegas@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Abstract

A sustainable society requires the recycling of greenhouse gases into useful products (e.g. CO₂ into CO and O₂). For this conversion process, low-temperature plasmas are essential, in interaction with solid-state electrolyzer separation membranes. Low-temperature plasmas are electrically-powered reactive gases with ideal conditions for gaseous conversion, while solid-state membranes can promote specific reactions and selectively induce the transport of certain species, thus potentially separating conversion products (e.g. CO and O₂). The merge of the two technologies is a novel approach with increasing attention, but the interaction between the plasma and these surface materials is still widely unknown.

The physics of low-temperature plasma reactors comes across different temporal and spatial scales and involves the interplay between different branches of physics: electromagnetism, fluid mechanics, statistical physics and gaseous and surface reactivities. An accurate description of the plasma-membrane system and of these media in general that allows predictive modelling and reactor optimization requires the development of multidimensional numerical models. The goal of this work is to engage in multidimensional continuum simulations of low-temperature plasmas. The first step is to learn the basics of CFD (computational fluid dynamics) and plasma fluid numerical modelling through a hands-on approach and in-house code development. Then, depending on the student's interests, an available numerical plasma code (e.g., SOMAFOAM, FEniCSx, SPARK) may be chosen or in-house coding may proceed to the development of a self-consistent plasma model. Subsequently, a simplified system will be defined to be used as a test-bed to study the capabilities and performance of the code. Depending on the available time, the model can be further developed to study real plasma-membrane systems with experimental validation. The project will be supervised by plasma modelers, within the cadre of wider projects developing technologies for sustainable gaseous conversion, such as Project PARADiSE - the Plasma RoAD to Solar fuEls, involving plasma reactor experiments. International collaborations are in place and research stays at laboratories in France, The Netherlands, Czech Republic, Italy, Japan and the USA, among other countries, are possible.

Goals

The goal of this work is to engage in multidimensional continuum simulations of low-temperature plasmas. The first step is to learn the basics of CFD (computational fluid dynamics) and plasma fluid numerical modelling through a hands-on approach and in-house code development. Then, depending on the student's interests, an available numerical plasma code (e.g., SOMAFOAM, FEniCSx, SPARK) may be chosen or in-house coding may proceed to the development of a self-consistent plasma model. Subsequently, a simplified system will be defined to be used as a test-bed to study the capabilities and performance of the code. Depending on the available time, the model can be further developed to study real plasma-membrane systems with experimental validation.

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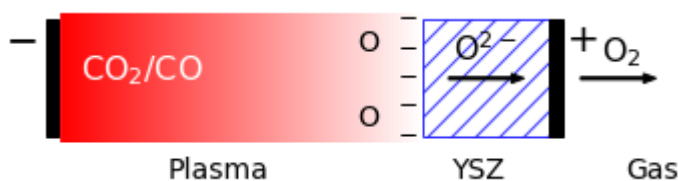
Title: Modelling the interaction between low-temperature plasmas and separation membranes

Supervisors: Pedro Viegas (pedro.a.viegas@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Abstract

A sustainable economy requires the recycling of greenhouse gases into useful products (e.g. CO₂ into CO and O₂). For this conversion process, low-temperature plasmas are essential, in interaction with solid-state electrolyzer separation membranes. Low-temperature plasmas are electrically-powered reactive gases with ideal conditions for gaseous conversion, while solid-state membranes can promote specific reactions and selectively induce the transport of certain species, thus potentially separating conversion products (e.g. CO and O₂). The merge of the two technologies is a novel approach with increasing attention, but the interaction between the plasma and these surface materials is still widely unknown.

In this project, the student will develop a numerical model to describe the plasma, the adsorption of plasma species (e.g. O) onto the surface, the formation of ions to be conducted at the surface (e.g. O²⁻) and the transport of ions within the material, for different operating conditions of practical interest. Such a model will allow us to study the interdependence between plasma and membrane parameters and analyze the fundamental interactions between plasma species and surface materials. The numerical model will start from an existing code of the research team for plasma kinetics, plasma-surface interactions and membrane reactions and will be further developed to study new phenomena concerning the separation membranes and their interaction with the plasma and different conditions of interest. Depending on the student's specific interest and the available time, the model may be developed within a global modelling approach or in a multidimensional fluid/kinetic framework. The project will be supervised by plasma researchers in close contact with surface experts, within the cadre of wider projects developing technologies for sustainable gaseous conversion, such as Project PARADISE - the Plasma RoAD to Solar fuEls. International collaborations and contacts with experimentalists are in place and research stays at laboratories in France, The Netherlands, Italy, Japan and the USA, among other countries, are possible.



Goals

In this project, the student will develop a numerical model to self-consistently describe the plasma, the adsorption of plasma species (e.g. O) onto the surface, the formation of ions to be conducted at the surface (e.g. O₂⁻) and the transport of ions within the material, for different operating conditions of practical interest. Such a model will allow to study the interdependence between plasma and membrane parameters and analyze the fundamental interactions between plasma species and surface materials.

Period: School year 2024/2025

Framework: PIC2/MSc thesis, internship

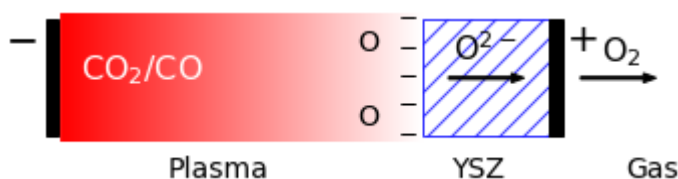
Title: Experimental characterization of the interaction between low-temperature plasmas and separation membranes

Supervisors: Pedro Viegas (pedro.a.viegas@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal, Olivier Guaitella (olivier.guaitella@lpp.polytechnique.fr), LPP/École Polytechnique, France and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Abstract

A sustainable economy requires the recycling of greenhouse gases into useful products (e.g. CO₂ into CO and O₂). For this conversion process, low-temperature plasmas are essential, in interaction with solid-state electrolyzer separation membranes. Low-temperature plasmas are electrically-powered reactive gases with ideal conditions for gaseous conversion, while solid-state membranes can promote specific reactions and selectively induce the transport of certain species, thus potentially separating conversion products (e.g. CO and O₂). The merge of the two technologies is a novel approach with increasing attention, but the interaction between the plasma and these surface materials is still widely unknown.

In this project, the student will work in the world-class laboratory Laboratoire de Physique des Plasmas (LPP), in France, to measure key parameters in novel plasma-membrane set-ups. The measurements should characterize the plasma, the adsorption of plasma species (e.g. O) onto the surface, the formation of ions to be conducted at the surface (e.g. O²⁻) and the transport of ions within the material, for different operating conditions of practical interest. Such measurements will allow us to study the interdependence between plasma and membrane parameters and analyze the fundamental interactions between plasma species and surface materials. Inclusively, the measurements will support the validation of new plasma-membrane models. The laboratory is equipped with a plasma-membrane set-up and with state-of-the-art diagnostics. The project will be supervised by experimental plasma researchers in close contact with surface experts and plasma modelers in Portugal, within the cadre of wider projects developing technologies for sustainable gaseous conversion, such as Project PARADiSE - the Plasma RoAD to Solar fuEls.



Goals

In this project, the student will work in the world-class laboratory Laboratoire de Physique des Plasmas (LPP), in France, to measure key parameters in novel plasma-membrane set-ups. The measurements should characterize the plasma, the adsorption of plasma species (e.g. O) onto the surface, the formation of ions to be conducted at the surface (e.g. O²⁻) and the transport of ions within the material, for different operating conditions of practical interest.

Period: School year 2024/2025

Framework: PIC2/MSc thesis, internship

Title: Feasibility study on the integration of Plasma Technologies into Mars ISRU systems

Supervisors: Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL, Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Non-equilibrium plasmas have shown significant potential in converting CO₂ from the Martian atmosphere into O₂ for astronauts to breathe or for landing vehicles as an oxidizer [1,2]. The process also produces CO which can be used as a low-quality fuel or transformed into methane if reacted with water. Preliminary assessments showed that the technology is easily scalable, requires small power input and yet featuring a high efficiency on Mars, compared to traditional ISRU systems like Solid Oxide Electrolysis Cells (SOEC) - the main component of the MOXIE system.

While plasmas look promising, any ISRU unit shall prioritise the minimization of mass, power and supplies from Earth to be viable on the long term [3]. During this project, we will seek to evaluate the feasibility of a plasma-based ISRU unit and its efficiency using back-of-the-envelope calculations. The project time line is divided into four steps:

- *Identifying areas where plasma technologies might be relevant and the plasma type:* Non-equilibrium plasmas are versatile with Earth applications ranging from agriculture to manufacturing and space. Mars' low-pressure atmosphere (600 Pa on average) gives non-equilibrium plasmas a major advantage. However, the efficiency will highly depend on the plasma configuration.
- *Assessing the cost of a plasma-based ISRU unit compared to current ISRU units, particularly MOXIE:* The cost of the ISRU units will be compared considering the materials or components that need to be transported from Earth and those that can be supported by Mars in-situ resources. Current estimations suggest plasma reactors would require between 25 – 100W with efficiencies that outperform the traditional means, but the subsequent subsystems might significantly impact the power needs and the total efficiency. The analysis shall provide a mass and a power budget and a breakdown of the estimated total efficiencies of the subsystems.
- *Defining a roadmap for implementing a plasma-based ISRU unit:* The final phase of the project shall involve a roadmap for testing and implementing the plasma-based ISRU unit. Recommendations shall focus on the critical bottlenecks to optimizing efficiency, a testing plan including laboratory, Martian analog experiments and qualifications test, and finally a suggested architecture of the Martian colony with the integrated system. Considerations shall include logistical and operational factors, emphasizing on maximizing in-situ resource use and minimizing Earth-supplied materials.

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

- [1] V. Guerra, T. Silva, and O. Guaitella, 'Living on mars: how to produce oxygen and fuel to get home', *Europhys. News*, vol. 49, no. 3, pp. 15–18, May 2018, doi: 10.1051/ePN/2018302.
- [2] L. G. McKinney, 'Plasma-based CO₂ Conversion for Mars ISRU', Thesis, Massachusetts Institute of Technology, 2024. Accessed: Jul. 01, 2024. [Online]. Available: <https://dspace.mit.edu/handle/1721.1/155377>
- [3] G. Sanders et al., *Mars ISRU for Production of Mission Critical Consumables - Options, Recent*

Studies, and Current State of the Art. 2015. doi: 10.2514/6.2015-4458.

Title: Experimental assemble of a microwave plasma for ISRU

Supervisors: Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IPFN/IST-UL, Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

The achievement of a manned-mission to Mars will mark the next frontier of discovery and the dawn of a new age in planetary exploration. Among the many scientific and technical challenges required to make this journey a reality, the harvesting of local resources at the site of exploration is of a special and mandatory importance. This approach is known as in situ resource utilization (ISRU) and it has the potential to enable humans to thrive beyond Earth, in a self-sufficient way, for extended periods of time. Over the past years the team at IPFN conducted several modeling studies targeted at demonstrating that the cold temperatures of Mars can preserve the asymmetric vibrations of CO₂, which accumulate energy for the molecular decomposition and subsequent oxygen production [1,2]. The feasibility of oxygen production on Mars through plasma technology has also been corroborated by several experimental campaigns – see e.g. [3]. To further advance plasma technology in the context of ISRU, this work will target the assembly of a plasma-based setup, exclusively dedicated to research of non-thermal microwave discharges operated under conditions of interest to the production of useful products in space. The laboratory will serve as a crucial platform to study key challenges associated with the use of plasmas in ISRU, namely related to plasma reactor weight reduction, chemical conversion and gas separation.

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

[1] V. Guerra, T. Silva, and O. Guaitella, ‘Living on mars: how to produce oxygen and fuel to get home’, *Europhys. News*, vol. 49, no. 3, pp. 15–18, May 2018, doi: 10.1051/epn/2018302.

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[3] P. Ogloblina et al., *Plasma Sources Sci. Technol.* 30 (2021) 065005.

Title: Towards the understanding of NO Production in N_2-O_2 Plasmas, sustained in presence of catalysts, with OD Kinetic Modeling and Experimental Validation

Supervisors: Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IPFN/IST-UL, Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

The achievement of a manned-mission to Mars will mark the next frontier of discovery and the dawn of a new age in planetary exploration. Among the many scientific and technical challenges required to make this journey a reality, the harvesting of local resources at the site of exploration is of a special and mandatory importance. At IPFN, our team has been at the forefront of groundbreaking research in this field. We have conducted several modeling studies that demonstrate how Mars' cold temperatures can preserve the asymmetric vibrations of CO_2 , storing energy for molecular decomposition and oxygen production [1,2]. This cutting-edge research has been supported by experimental campaigns confirming the feasibility of producing oxygen on Mars through plasma technology [3]. To further advance plasma technology in the context of ISRU, this work will target the assembly of a microwave plasma-based setup, operated under conditions of interest to the production of useful products in space. This system, designed to operate under conditions relevant to space exploration, will be essential for addressing key challenges, such as reducing reactor weight, optimizing chemical conversion, and improving gas separation.

Period: School year 2024/2025

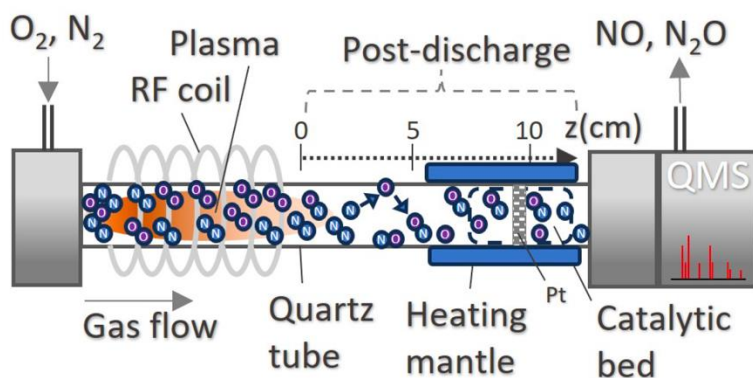
Framework: PIC1, PIC2/MSc thesis, Internship

- [1] V. Guerra, T. Silva, and O. Guaitella, 'Living on mars: how to produce oxygen and fuel to get home', Europhys. News, vol. 49, no. 3, pp. 15–18, May 2018, doi: 10.1051/epn/2018302.
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Supervisors: Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IPFN/IST-UL, Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

The transition from reliance on fossil fuels to the integration of renewable energy has become an urgent and essential pursuit, driven by the need to confront the challenges of climate change. Among the strategies designed to address this, the Power-to-X (P2X) approach plays a critical role in reducing carbon emissions and stabilizing power supply amid the intermittency of renewable energy sources. Within P2X, renewable electricity serves as a key enabler for the transformation of elemental molecules such as CO_2 and N_2 into high-energy compounds and valuable chemical feedstocks. While CO_2 conversion is often associated with waste recycling and the generation of carbon-neutral fuels via the Fischer–Tropsch process, N_2 conversion is integral to nitrogen fixation and the production of nitric acid (HNO_3), a vital source of nitrates used in plant fertilizers. This work focuses on exploring the potential of non-thermal plasmas to promote efficient nitrogen fixation in various N_2 - O_2 mixtures, with a particular emphasis on the role of catalysts under different oxygen concentrations. Recent advancements in simulation tools will be leveraged to describe the volume chemistry of non-thermal discharges, coupled with a mesoscopic model of reactor surface dynamics, accounting for adsorption sites and elementary surface phenomena [1]. Several reactor configurations will be investigated, including low-radiofrequency (13.56 MHz) discharges at 5 mbar pressures, as well as dielectric barrier discharges at atmospheric pressure.



Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

[1] T. Silva et al., *J. Phys. Chem. A* 2024, 128, 7235–7256.

Title: Electron dynamics and heavy-particle kinetics in atmospheric pressure air plasmas

Supervisors: Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IPFN/IST-UL, Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Atmospheric pressure plasmas are of great interest due to their simple operation, reduced processing cost, and the possibility of the application of plasma to samples that are not compatible with low-pressure conditions, in particular in the rapidly growing fields of plasma medicine and plasma agriculture. This work proposes a joint modeling and experimental study of air-containing atmospheric discharges aiming at a precise determination of the plasma parameters, namely electron density and electron temperature. Research efforts will be targeted at developing a plasma-based kinetic scheme for ns pulse jet discharges (see figure 1) sustained at atmospheric pressure and with gases mixtures containing Helium with small admixtures of CO₂. The work will be developed in the framework of a collaboration between the Instituto Superior Técnico, where the models will be developed (based on the LisbOn KInetics (LoKI) simulation tool [1,2]), and the Nagoya University where the experimental work (see e.g. [3]) will be carried out. The experimental campaign will be supervised by Dr. Nikolay Britun.

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

References:

- [1] A. Tejero-del-Caz et al., *Plasma Sources Sci. Technol.* **28** (2019) 043001.
- [2] A. Tejero-del-Caz et al., *Plasma Sources Sci. Technol.* **30** (2021) 065008.
- [3] N. Britun et al., *Plasma Sources Sci. Technol.* **31** (2021) 125012.

Title: Development of novel methods based on machine-learning and graph-theoretical approaches for the understanding of plasmas.

Supervisors: Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IPFN/IST-UL, Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Plasmas play a vital role in a broad spectrum of industrial, environmental, and technological applications. To deepen the understanding of plasma chemistry, it becomes essential to develop precise yet simplified kinetic models. In this context, research at N-PRiME within IPFN has concentrated on advancing methods to analyze the key mechanisms that govern plasma behavior – see e.g. [1]. To create a more robust and adaptable platform for studying, reducing, and simplifying plasma kinetic schemes, the integration of innovative techniques becomes crucial. This study proposes the use of machine learning-based methods and graph-theoretical analysis as novel tools to extract critical insights from complex plasma chemistry. By harnessing the structural properties of chemical networks, these methods promise to streamline and enhance the understanding of plasma reactions. The work will benefit from a collaboration between Instituto Superior Técnico and Seikei University, led by Dr. Tomoyuki Murakami (author of the study in [2]).

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

References:

- [1] L. Terraz et al., *J. Phys. Chem. A* 124 4354 (2020)
- [2] T. Murakami and O. Sakai, *Plasma Sources Sci. Technol.* 29 (2020) 115018



Title: Fast multipole method for plasma physics

Supervisor: Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

The numerical solution to N-body problems in gravitation or electrostatics has traditionally been obtained via particle-in-cell methods (PIC), since direct evaluation of all pairwise interparticle forces requires $O(N^2)$ operations and is computationally too expensive.

An alternative to PIC are hierarchical solvers, which use tree data structures and lumped-force approximations, making simulations feasible in $O(N \log N)$ operations. The purpose of this thesis is to explore the use of the fast multipole method (FMM) in electrostatic particle simulations in plasma physics and compared FMM with the PIC methodology.

Period: School year 2024/2025

Framework: PIC2/MSc thesis

Title: Machine learning for optimization of plasma-assisted conversion of CO₂

Supervisors: Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL, Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Plasma technologies are very promising for green conversion of CO₂ into value-added products and energy storage in liquid fuels. However, accurately predicting plasma properties presents a significant challenge, given the inherent complexity of the underlying chemistry models and the uncertainties surrounding several input parameters. In particular, the predictions critically depend on reaction rate coefficients that are often poorly known and are tuned with time-consuming trial-and-error approaches. This work aims at using machine learning to optimize a model for plasma-assisted conversion of CO₂ and to find the corresponding reaction rate coefficients. Additionally, automated processes will be explored to identify the most relevant features of the reaction set and to model uncertainties in deep learning models, as to identify influential mechanisms and to provide an estimate of confidence for the model outputs. Experimental data for model validation will also be obtained.

Research goals:

- Use deep learning models to learn and optimize the set of reaction rate coefficients in predictive plasma models
- Use dimensionality reduction techniques to identify the most relevant species and mechanisms
- Model uncertainties in the neural network and estimate confidence intervals for the outputs
- Obtain experimental data for model validation

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

Title: Transfer learning for plasma CO₂ Conversion on Mars

Supervisors: Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL, Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Non-equilibrium plasmas have shown significant potential in converting CO₂ from the Martian atmosphere into O₂ for astronauts to breathe or for landing vehicles as an oxidizer [1,2]. The process also produces CO which can be used as a fuel directly or transformed into methane if reacted with water. Preliminary assessments showed that the technology is easily scalable, requires a small power input, and yet features a higher efficiency than traditional ISRU systems such as the MOXIE system.

However, optimizing this process is challenging due to the complex plasma chemistry, particularly the lack of precise knowledge about some reaction rate coefficients and the interactions between various species. In this context, Machine learning (ML) might offer a promising way to enhance the efficiency of CO₂ conversion by identifying key plasma-chemical pathways and optimizing reaction rate coefficients.

This proposal will look into the application of transfer learning to build a surrogate model for Mars plasma aided CO₂ conversion. The idea behind transfer learning is that we can pre-train a model on both synthetic data generated by the LoKI chemistry model developed by IPFN. Then tune the acquired “knowledge” based on experimental data. Specifically, the idea is to explore the possibility to provide a hybrid learning methodology where we can use the experimental data as high confidence data while relying on synthetic data to extend to unknown values.

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

Title: Data-driven and physics-informed measurement of rate coefficients for plasma processes

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The "Report on Science Challenges and Research Opportunities for Plasma Applications in Microelectronics", issued by the US Department of Energy, Office of Science Fusion Energy Sciences, from January 2023, identifies the "Develop fundamental data and centralized databases to enable comprehensive low temperature plasma diagnostics and modelling" as "Priority Research Opportunity" (PRO). One of the "Scientific questions" enumerated within this PRO is "How can machine learning enable faster development of reliable reaction mechanisms for plasma chemistry and plasma-surface interaction? What experimental data would be needed to help with this effort?"

The N-PRiME group of IPFN has a vast work on the development of reaction mechanisms for plasma chemistry and on the identification and generation of the required experimental data, albeit without resorting to machine learning. This work capitalizes on the expertise of ISR in machine learning and the competences of IPFN to address the scientific question stated above.

The goal of this project is to predict rate coefficients -and potentially cross sections or even Einstein coefficients- based on available experimental data, using a surrogate machine learning model. The problem can be stated as follow: while the dominant reactions within the plasma for a given range of pressure and temperature are known, the rate coefficients for some reactions remain undetermined for some gas mixtures. Access to experimental measurements (reduced electric field, gas temperature, metastable densities, emission spectra ...) might provide a potential way to solve this inverse problem and help determine missing rate coefficients: We might extract the missing rate coefficients, the cross sections or Einstein coefficients for the missing processes based on the experimental values, assuming that the plasma is described by the set of reaction given as an input. Stated in this form, the problem can be understood as a multi-dimensional least-squares optimization problem with $N > 100$, where the goal is to minimize the difference between model predictions and experimental data across the parametric space defined by the set of the missing rate coefficients.

To achieve this, we will rely on Machine Learning (ML) and Physics-Informed Machine Learning (PI-ML) will be incorporated to impose physical constraints, ensuring that the models respect the fundamental physical governing plasma behaviour. Furthermore, uncertainty quantification will be implemented to enhance the reliability of the models, using Bayesian optimization or Gaussian processes. These methods will provide confidence intervals for the model's predictions, allowing for a more robust analysis of the plasma chemistry. Finally the project will look into the impact of adding a new measurement of a missing rate coefficient on the overall prediction of the model, i.e. how the measurement of missing rate coefficient would improve or degrade the predictions of the model.

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

Title: Machine-Learning lumping methodology for kinetic schemes reduction for CO₂ conversion on Mars

Supervisors: Tarek Ben Slimane (tarek.b.slimane@tecnico.ulisboa.pt), IPFN/IST-UL and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IPFN/IST-UL, Portugal

Non-equilibrium plasmas have shown great potential in converting CO₂ from the Martian atmosphere into O₂, which can be used by astronauts or as an oxidizer for landing vehicles. The process also produces CO, which can either be used as a fuel or converted into methane when reacted with water. Early evaluations indicate that plasma-based technology is highly scalable, requires less power input, and offers higher efficiency compared to traditional ISRU systems like the MOXIE system.

Despite the promise of plasma technology, the current kinetic models are highly complex due to the large number of species involved in the Martian atmosphere. One way to simplify this complexity is through lumping strategies, where species with similar characteristics are grouped into one effective level. For example, excited states close to ionization thresholds, as well as vibrational and rotational levels, can be lumped into one single effective level. This significantly reduces the number of levels needed for simulation.

Machine Learning (ML) and data-driven models can play a key role in accelerating these simulations by treating the lumped levels as a surrogate model within a neural network. This approach would allow us to maintain the most important physics while reducing computational time. Additionally, it lowers the common critic to learning models becoming a "black box" since we still track how the lumped levels interact with other species in the plasma, allowing us to judge if the behaviour is realistic and correct. This approach to lumping is quite unorthodox since usually effective levels are created analytically from the balance equations, which sometimes when the number of species and processes is high, it can become very challenging.

The project aims to address these challenges using the kinetic schemes developed at IPFN from the LoKI tool (LisbOn KInetic). It will be divided into four key milestones by increasing complexity:

- Lumping radiative states: grouping radiative states in pure argon discharges at low pressures.
- Lumping vibrational levels of oxygen: Simplifying vibrational levels of the oxygen molecule in pure oxygen discharges at low pressures.
- Lumping vibrational levels of CO₂: Reducing the complexity of vibrational levels in pure CO₂ discharges at low pressures.
- Mixed Argon/CO₂ simulation: Testing a mixture of Ar/CO₂.

The accuracy and speed-up of the simulations will be systematically evaluated at each step. We will try at each step of the project to enforce Physics Informed Machine Learning (PI-ML) so that to integrate physical constraints into the ML mode, ensuring that important plasma behaviours as well as atomic and molecular physics are preserved. Cross section and rate coefficients comparison.

Period: School year 2024/2025

Framework: PIC1, PIC2/MSc thesis, Internship

Title: Towards Carbon Neutrality: Modeling and Assessing Plasma-Based Nitrogen Fertilizer Production

Supervisor: Júlio Henriques (julio.henriques@tecnico.ulisboa.pt), IPFN-IST/Univ. Lisbon, Portugal

Abstract

Traditional methods of producing nitrogen-based fertilizers are increasingly unsustainable, consuming significant amounts of energy and contributing to approximately 1.4% of global CO₂ emissions. With nitrogen fertilizer production accounting for around 2% of global energy use and 5% of natural gas consumption, finding a sustainable alternative is crucial, especially in light of the European Union's goal for carbon neutrality by 2050.

This research explores an innovative plasma technology developed at IPFN, patent pending, that utilizes plasma to create nitrogen fertilizers composed of nitrates and ammonium. By injecting a mixture of natural nitrogen, oxygen, and hydrogen into microwave plasmas, this method dissociates molecules and produces reactive species, ultimately forming these essential nutrients. The process relies solely on electricity sourced from renewables, promoting energy sustainability and minimizing environmental impact.

To better understand the processes leading to nitrogen-based fertilizer formation, a 2D plasma model has been developed, incorporating a self-consistent description of electron kinetics, heavy-species kinetics, gas dynamics, and wave electrodynamics.

Goals

- **Literature Review:** Investigate recent advancements in plasma-based fertilizer production, identifying current challenges and gaps in the research.
- **Plasma Process Modelling:** Create computational models to simulate the interactions within the plasma, focusing on the dissociation processes and fertilizer synthesis.
- **Environmental Impact Assessment:** Compare the sustainability of plasma-based nitrogen fertilizer production with conventional methods, highlighting its potential benefits.

This research aims to deepen our understanding of how plasma technology can revolutionize sustainable fertilizer production, integrating concepts from plasma physics with practical solutions that can significantly benefit agriculture and the environment.

Period: Flexible

Framework: PIC2/MSc thesis, among other possible frameworks.

Title: Hall Thruster Modeling and Performance Optimization for Advanced Electric Propulsion Systems

Supervisors:

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Prof. Paulo Sá, Faculty of Engineering/Univ. Porto, Portugal

Prof. Mario J. Pinheiro, Instituto Superior Técnico /Univ. Lisbon, Portugal

Abstract

Hall thrusters are pivotal in modern space propulsion, offering efficient, high-performance solutions for satellite maneuvering and deep-space missions. The proposed study focuses on the comprehensive modelling of Hall thrusters to enhance their performance for various propulsion applications. Utilizing advanced computational techniques such as Particle-In-Cell (PIC) and Direct Simulation Monte Carlo (DSMC) methodologies, this study simulates complex plasma dynamics within the thruster and its plume, employing Xenon and Argon as primary propellants. Simulations are performed using COMSOL Multiphysics® to model particle interactions, including first and second ionization processes.

The simulation results will be validated against experimental data and existing models developed by Kawashima and Allis, providing critical insights into optimizing thruster efficiency, thrust and other parameters and physics predicting ion trajectories and energy distributions accurately.

Goals

- **Literature Review:** Conduct an in-depth Investigation of existing literature to assess prior knowledge and identify specific gaps in research.
- **Performance Enhancement:** Develop and refine models to optimize thrust and efficiency under various operating conditions.
- **Advanced Simulation Techniques:** Employ PIC and DSCM methods to simulate the intricate plasma dynamics within the thruster and its exhaust plume.
- **Incorporate Established Models:** Validate and refine existing frameworks by comparing results with Kawashima and Allis's models.
- **Ionization Analysis:** Examine first and second ionization processes to enhance plasma generation and stability, improving thruster operation.
- **Experimental Correlation:** Align simulation outcomes with experimental data to ensure practical applicability and reliability of the models.

In summary, this research aims to optimize Hall thrusters, enhancing their efficiency and expanding their applications in space exploration and satellite operations.

Period: Flexible

Framework: Internship

Title: Control and Automatization of Plasma Reactor for the Synthesis of Nanostructures

Supervisors:

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Abstract

Plasma Engineering Laboratory (PEL) has developed a disruptive plasma method for the synthesis of carbon-based nanostructures. At the heart of this novel technology is a pre-industrial prototype, currently at Technology Readiness Level (TRL) 5, that combines both off-the-shelf and custom-made equipment, allowing the ignition and maintenance of the high energy density non-thermal plasma that fosters the selective growth of various types of nanostructures. Currently, to operate the device, a user must interact with the control modules of each individual subsystem, such as the power supply, flowrate controllers, heat dissipation modules, etc. On the path towards an industrial machine, these systems need to be further integrated, and their controls centralized in a single user-friendly console with automation capabilities in order to make the operation of the prototype accessible to the non-specialized user.

Goals

The goal of this work is to develop a centralized control and automation framework. Depending on the candidate's profile and the framework, this will include some or all of the following tasks:

- Familiarization with fundamental concepts of surface wave-driven plasma sources
- Operate of the PEL large scale prototype
- Develop communication modules to monitor and control each of the subsystems using a computer (e.g.: LabView, EPICS)
- Develop software routines to ignite and maintain the plasma.
- Integrate the control modules and the operational routines in a single PC-like device

Period: (from February to July, scholar year 2024/2025)

Framework: (PIC1, PIC2/MSc thesis, internship, other)

Title: Electromagnetic Performance Assessment of Novel Graphene-based Nanomaterials

Supervisors:

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Abstract

Graphene-based nanomaterials hold great potential for Electromagnetic Shielding applications by combining low weight, stability and exceptional EM absorption performance. Using IPFN developed plasma-enabled synthesis technology, a large array of graphene-based nano hybrids can be selectively synthesized in a single-step at atmospheric pressure using a single machine. To optimize both the production protocols and the properties of the synthesized materials it becomes fundamental to quickly and precisely measure the EM absorption, transmission and reflection coefficients of multiple produced samples in a laboratorial environment. To do so, a testbench composed by a state-of-the-art Vector Network Analyser (VNA) and waveguide elements suitable for each of the frequency bands under investigation can be employed.

Goals

The goal of this assignment is to assemble and operate a testbench to determine the EM performance assessment of novel nanomaterials produced at PEL. Depending on the candidate's profile and the framework, this will include some or all of the following tasks:

- Familiarization with fundamental concepts of Electromagnetic waves propagation in different media.
- Assemble a testbench featuring a state-of-the-art 100kHz-26.5GHz VNA.
- Use the assembled testbench to measure the Scattering Parameters (S-parameters) of the nanomaterials.
- Analyse the measurements and determine the EM performance of the novel nanohybrid samples produced at PEL.

Period: (from February to July, scholar year 2024/2025)

Framework: (PIC1, PIC2/MSc thesis, internship, other)

Title: Graphene-Metal Hybrids with Enhanced Properties for Hydrogen Storage

Supervisor: Ana Amaral Dias (ines.vieitas@tecnico.ulisboa.pt), IPFN/IST, Portugal

Abstract

The Hydrogen RoadMap Europe report indicates that by 2050 hydrogen could provide up to 25% of the total energy needs. Nevertheless, hydrogen's potential has not been reached completely due to storage challenges. Among the storage methods the solid-state storage of hydrogen has shown promising results and is more reliable in terms of transportation and safety. Presently, the concept of storing hydrogen in materials in a reversible manner is considered as a long-term solution for hydrogen storage. Most of the storage systems are being actively explored and the creation of a solution capable of holding strong enough H₂ adsorption for stable thermodynamic state and weak enough to release H₂ at acceptable temperature, remains a big challenge to overcome. Meanwhile, currently available fabrication techniques of carbon-metal-based composites suffer from many limitations, including high energy consumption, lengthy processing times, and difficulty in tailoring the material's properties precisely for hydrogen storage, namely non-uniform nanoparticles coverage, low density, weak interfacial interaction, etc. These issues lead to low material quality. Therefore, disruptive plasma-enabled assembly pathways will be employed to accomplish controllable atom-by-atom design of matter at nanoscales via exclusive plasma mechanisms to rule the quanta and localization of energy and matter at atomic scale [1-2]. This work will lead to significant advancements in the practical application of hydrogen storage systems, contributing to sustainable energy solutions.

Goals

Optimize exiting plasma-assisted methods at PEL for the fabrication of graphene-metal-based hybrids tailored for hydrogen storage. Optimize plasma parameters (e.g., power, gas flow rates, pressure, etc) to control particle size, nanoparticles distribution in the graphene matrix, and structures stability.

Enhance hybrids hydrogen storage capacity, synthesising hybrids with high hydrogen adsorption and desorption capacities. Focus on improving material porosity, surface area, and hydrogen-metal interaction to enhance storage performance.

Familiarization with plasma environment and materials characterization techniques available at PEL (i.e., OES, FTIR, XRD, etc) and in collaborating institutions (i.e., SEM, EDS, TEM, XPS, NEXAFS, etc) to better understand and optimize the key properties that influence hydrogen storage capacity.

Period: 2024/2025

Framework: PIC2, MSc thesis, internship

[1] A. Dias et al, Applied Materials Today 36 (2024) 102056. <https://doi.org/10.1016/j.apmt.2024.102056>

[2] D. Tsyganov et al, Materials 2020, 13:18 (2020) 4213. <https://doi.org/10.3390/ma13184213>

Title: Microwave plasmas for synthesis of advanced materials for Electromagnetic Wave Shielding and Absorption

Supervisors:

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Abstract

Graphene and graphene-based composite materials are of great interest for numerous applications due to their exceptional properties. The common synthesis methods of such materials however are lengthy and complex chemical processes which require the use of toxic agents and very often lead to low quality materials. Alternatively, a plasma-based method for synthesis of advanced 2D nanostructures is an environmentally friendly technique (without use of catalysts, acids etc.), which allows control over the synthesis process. In fact, plasmas can be used to produce not only high-quality graphene but also graphene composites in a single step and in a controllable manner. Depending on the targeted application the plasma parameters can be tailored to foster synthesis of planar graphene or particle-like carbon, as well as graphene-metal composites by adding metal microparticles in the plasma medium.

One emerging application of novel advanced graphene-based materials is for electromagnetic (EM) shielding. EM radiation, due to increased use of electronic and communication devices, is a source of pollution that can disrupt normal communication, but also can pose a potential threat to human health. Graphene-based composites are promising candidates for EM shielding, featuring losses from absorption or multiple reflection effects.

Goals

The major goal of the project is to fabricate graphene-based composites with metal oxide nanoparticles by using microwave plasma-based method (developed in Plasma Engineering Laboratory PEL), which present high EM shielding performance in broad frequency range (2-20 GHz). It has been shown that one single material cannot satisfy all the shielding aspects (thickness, broadband response, volume, absorption properties, etc.) required for the best efficiency. Therefore, efforts are directed towards developing composites consisting of both magnetic and electric components, providing better shielding efficiency and enhanced EM absorption performance. Incorporating magnetic metal nanoparticles (e.g.: Fe, Co, Ni) into graphene can increase the extra magnetic loss and polarized interfaces and regulate the impedance mismatching via tuning the electromagnetic parameters.

The candidate will be responsible for synthesis of graphene structures decorated with FeOx nanoparticles, using the existing microwave plasma setup(s). The influence of the operating plasma parameters (microwave power, precursor type and flow, flowrate of metal nanoparticle etc.) will also be studied. The synthesized composite materials will be characterized by X-ray diffraction (XRD) technique.

Furthermore, different light weight and easy to process polymer materials such as polyurethane, polyethylene, epoxy etc. will be tested as a matrix for the created graphene-metal composites.

In the frame of this project the candidate will gain knowledge about microwave plasma device and its operation, the plasma-nanoparticles synthesis process, XRD characterization technique and experimental plasma science in general. In addition, he/she will get hands-on practice of operation

of important techniques and methods:

- Operation of microwave plasma system at atmospheric pressure conditions
- Technology of graphene-based composites synthesis by plasma method
- XRD characterization

Period: (from February to July, scholar year 2024/2025)

Framework: (PIC1, PIC2/MSc thesis, internship, other)

Title: Microwave plasmas for synthesis of nitrogen-doped graphene with low SEY

Supervisors:

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Abstract

Materials with low secondary electron yield (SEY), defined as average number of secondary electrons emitted per single incident electron, are of great interest for modern technologies, such as space applications (e.g. telecommunication satellites) and particle accelerators. In the latter, for instance, secondary electron emission can lead to formation of electron clouds which affect particle beam trajectories and introduce beam instabilities.

Free-standing graphene structures produced in Plasma Engineering Laboratory (PEL) by microwave plasma method were studied as potentially low SEY materials in collaboration with CEFITEC, Universidade Nova de Lisboa. Chemically inert graphene coatings obtained by electrophoretic deposition were prepared. Additionally, doping of graphene by foreign atoms, such as nitrogen, modifies its electronic properties, leading to further decrease of SEY.

Plasma Engineering Laboratory's developed plasma-based process of advanced 2D nanostructures synthesis is an eco-friendly and energy saving method that allows controllable production of high-quality graphene and nitrogen-doped graphene at a single step process and atmospheric pressure conditions.

Goals

The major goal of the project will be to fabricate nitrogen-doped graphene using microwave plasma-based method, for low SEY materials. Different precursors for carbon and nitrogen will be used (such as ethanol, methane, acetonitrile, ammonia, methylamine) to investigate the nitrogen doping levels and configurations (pyridinic, pyrrolic, graphitic etc.) and their influence on the SEY. The major task of the candidate will be to prepare different nitrogen-doped graphene samples, finding appropriate plasma parameters for synthesis of planar structures.

Material characterization is planned by X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM) analyses.

Further treatment of the as produced N-graphene samples will proceed jointly with the colleagues from CEFITEC, thanks to the firm collaboration established previously. This will include measurement of the SEY and X-ray Photoelectron Spectroscopy of the free-standing graphene samples, and of the corresponding coatings deposited on copper and stainless steel.

In the frame of this project the candidate will gain knowledge about microwave plasma discharges, the plasma-nanoparticle synthesis process, XRD characterization technique and experimental plasma science in general. In addition, he/she will get hands on practice of operation of important techniques and methods:

- Operation of microwave plasma system at atmospheric pressure conditions
- Technology of N-graphene synthesis by plasma method



- XRD characterization
- SEM analysis

Finally, the candidate will have the opportunity to collaborate with colleagues from another institution, which will further widen his/her scientific network.

Period: (from February to July, scholar year 2024/2025)

Framework: (PIC1, PIC2/MSc thesis, internship, other)