Shaping Energy for a Sustainable Future

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Code:
Project:
Area leader: Prof. Joan Ramon Morante
Group: Nanoionics and Fuel Cells
Group leader: ICREA Prof. Albert Tarancón Rubio

Project title / job position title
PhD Position, High-fidelity multiphysics modelling of solid oxide fuel cells and electrolisers

Context and Mission

The hydrogen vector is one of the most promising candidates to lead the energy transition towards a low-carbon society, which will take place within the next decade. Green hydrogen is generated from water and renewable electricity in an electrolyser. This renewable hydrogen can be stored and distributed for later use in highly efficient electrochemical systems such as fuel cells. The most efficient electrolyzers and fuel cells are based on Solid Oxide Cells (SOCs) operating at high temperatures. These novel technologies for electrolysis and power generation are called Solid Oxide Electrolysis and Fuel Cells (SOFCs and SOECs), respectively. SOFC/SOEC technologies involve multiple physical and chemical phenomena ranging from thermo-fluidics occurring at the cm-scale to electrochemistry taking place at the nanoscale. This multi-physics multi-scale complexity makes such devices extremely challenging from the simulation point of view while, at the same time, makes simulation outputs highly valuable to predict and design real operating systems.

The research activities will be conducted within a collaboration framework between the Propulsion Technologies Group at CASE Department of the Barcelona Supercomputing Center (BSC) (www.bsc.es) and the Nanoionics and Fuel Cells group (www.atlab.es) from the Catalonia Institute for Energy Research (IREC, www.irec.cat). The BSC team is a multidisciplinary group with researchers from all disciplines and with strong background in Computational Fluid Dynamics (CFD) and advanced software generation with High-Performance Computing (HPC). IREC is an international leader on SOFC/SOEC technologies with their own SOFC/SOEC technology, developed in collaboration with Spanish companies, and world-class facilities for the fabrication and characterization of SOC stacks and systems. These facilities will be used for testing the most advanced SOFC/SOEC technology and the generation of data for model validation.

Key duties
The research project is focused on the development of a high-fidelity multiphysics model of solid oxide fuel cells and solid oxide electrolysers (SOFCs and SOECs) using HPC-based technologies. More specifically, it is focused on the investigation of 3D effects in SOFC/SOEC using high-fidelity simulations.

The candidate will be located at BSC, but with continuous interactions with the IREC team. The PhD includes the development of a 3D model of the SOFC/SOEC, participation in measurement campaigns at IREC and cross-validation with the experimental data.

Requirements
Education
The candidate should hold a MSc Degree in Chemistry, Physics, Mechanical Engineering, or Aerospace with background in fluid mechanics and thermal systems. Solid background on Materials Science will be positively evaluated. Basic knowledge of electrochemical phenomena will be appreciated.

The candidate should fulfill the requirements to be enrolled in the Computational and Applied Physics PhD Program (https://doctorat-fcia.postgrau.upc.edu/es/informacion-general/profesorado) from the Universitat Politècnica de Catalunya.

Essential knowledge
General knowledge on fluid mechanics, chemistry, thermodynamics, electrochemistry, numerical methods are expected.

Additional knowledge
Computational skills and parallel programming for HPC are not necessary, but will be considered an asset.

Competences
- Ability to work independently and make decisions.
- Good communication and team-work skills to work in a multidisciplinary team.
- Fluency in English is essential, Spanish is welcome.

Application
The application should include:
- CV English, motivation letter and 2 support letters
- Starting date: 01/02/2022 - 28/02/2022
- Only online applications will be considered:
  - https://www.bsc.es/join-us/fellowships/41821caseptr1
- Deadline: 31/01/2022

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