

Pos-doc Materials Screening and First-principles
Calculations - REF 23PDR230
University of São Paulo

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Posted Apr. 5, 2024, set to expire Aug. 5, 2024

Job Title Pos-doc Materials Screening and First-principles Calculations - REF 23PDR230
Department Mechanical Engineering
Institution University of São Paulo
Sao Paulo, Sao Paulo, Brazil

Date Posted Apr. 5, 2024

Application Deadline Apr. 30, 2024

Position Start Date May 2024

Job Categories Post-Doc

Academic Field(s) Mechanical Engineering
Material/Metallurgy
Engineering Physics
Engineering Mechanics
Computer Science
Chemical/Petroleum
Engineering - Other

Job Website <https://sites.usp.br/rcgi/opportunities/>

Apply Online Here <https://docs.google.com/forms/d/e/1FAIpQLSfV4KkheEQeMJKiDnkVkoQIDm5pvKU28bFJR5uM>

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**Job
Description**

Project title:

Post-Doctoral Opportunity in Materials Screening and First-principles Calculations for Heterogeneous Catalysis and Fuel Cells to Produce hydrogen

Research theme area:

Fuel Cells, Ethanol Reforming, Hydrogen Production, Machine Learning, Density Functional Theory

Abstract:

The candidate will collaborate with researchers from the project 83 of the FAPESP-Shell Research Centre for Greenhouse Gas Innovation of POLI-USP at the University of São Paulo. Summary of the program and projects can be found at the RCGI website (<https://sites.usp.br/rcgi/>).

A successful candidate will combine machine learning and first-principles calculations to investigate materials for heterogeneous catalysis and electrochemical catalysis reactions, specifically focusing on the steam reforming of ethanol to produce hydrogen selectively. This position offers a unique opportunity to employ both methodologies to contribute to cutting-edge advancements in solid oxide fuel cells and the development of next-generation energy technologies. This position allows the candidate to apply for and develop an internship research period at Imperial College London.

Description:

The applicant will contribute in line with the main objectives of the project:

1. Employ advanced computational techniques and machine learning algorithms to identify and assess materials suitable for the catalysis in direct ethanol solid oxide fuel cells, focused on the steam reforming of ethanol.
2. Conduct First Principles calculations to investigate and describe the mechanisms of catalysed reactions, including steam reforming of ethanol.

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3. Collaborate closely with a multidisciplinary team of researchers to integrate your findings into developing solid oxide fuel cells running on ethanol.

Requirements to fill the position:

This project would be well-suited to a highly motivated candidate requiring Programming skills, experience in machine learning and DFT and proficiency in English are required.

- The postdoc candidate should hold a PhD in Physics, Chemistry, Computation, Materials Science or Engineering.

INFORMATION ABOUT FELLOWSHIP:

This Postdoc fellowship is funded by FAPESP. The fellowship will cover a standard maintenance stipend of R\$ 9,047.40 (Reais) per month.

MORE INFORMATION:

<https://sites.usp.br/rcgi/opportunities/>

Position: **Post-Doctoral Fellowship REF: 23PDR230**

[Access here](#) AND APPLICATION AT REF**Post-Doctoral REF.:23PDR230**

Contact Information

Please reference Academickeys in your cover letter when applying for or inquiring about this job announcement.

Contact RCGI
Human Resources
University of São Paulo
Av Prof Mello Moraes, 2231
Cidade Universitaria - Butanta
Sao Paulo, Sao Paulo 05508-030
Brazil

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Contact E-mail rcgi.opportunities@usp.br