Post-Doctoral Opportunity in Materials Screening and First-principles Calculations - REF.: 24PDR285
University of São Paulo

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Job Title	Post-Doctoral Opportunity in Materials Screening and First-principles Calculations - REF.: 24PDR285
Department	Engineering
	https://sites.usp.br/rcgi/
Institution	University of São Paulo
	São Paulo, São Paulo, Brazil
Date Posted	Jun. 11, 2024
Application Deadline	Jun. 28, 2024
Position Start Date	Jul. 1, 2024
Job Categories	Post-Doc
Academic Field(s)	Mechanical Engineering
	Engineering Physics
	Engineering Mechanics
	Engineering - Other
Job Website	https://sites.usp.br/rcgi/opportunities/
Apply Online Here	https://docs.google.com/forms/d/e/1FAIpQLSeTRWuw1b6jFfAu7mW4_DXsues8CSCv7ki7sxNq1m_pyBpLg/viewform
Apply By Email	

**Job
Description**

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.
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:

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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.: 24PDR285**

Access here AND APPLICATION AT REF**Post-Doctoral REF.: 24PDR285**

Contact Information

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

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