



## RESEARCH SCHOLARSHIP OPPORTUNITY

<b>Position reference number</b>		<b>Deadline for application</b>	20/12/2024
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<b>Institution</b>	Universidade de São Paulo
<b>Department</b>	Naval/Chemistry and Physics
<b>Supervisor</b>	Gustavo Assi/ Caetano Miranda

<b>Funding source</b>	FAPESP	<b>Type</b>	Postdoctoral researcher (PD)
<b>Duration (months)</b>	24	<b>Hours/week</b>	40
<b>Monthly stipend</b>	R\$ 12000, 00 (BRL Brazilian Reais)		
<b>Workplace</b>	Escola Politécnica, Instituto de Química e Instituto de Física, Universidade de São Paulo, Cidade Universitária, São Paulo SP, Brasil		
<b>Planned start date</b>	january 2025		

<b>Project title</b> Development of porous adsorbent materials based on Metal-Organic and Covalent-Organic Frameworks for transport and storage of H <sub>2</sub> and CO <sub>2</sub> .	<b>Título do projeto</b> Desenvolvimento de materiais adsorventes baseados em redes metalorgânicas para transporte e estocagem de H <sub>2</sub> e CO <sub>2</sub>
<b>Research theme</b> Computational methodologies	<b>Tema de pesquisa</b> Metodos computacionais
<b>Project abstract</b> The objective of this project is the development and study of materials with enhanced potential for adsorption/storage of H <sub>2</sub> , CO <sub>2</sub> and other gases of interest, based on metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs). These highly porous materials are capable of absorbing, retaining, separating, and releasing molecules in/from their porous networks. The core innovation of the project is to use Materials Informatics by combining multiscale molecular simulations, machine learning, and topology optimization to accelerate the screening selection and design optimized morphologies to enhance the selectivity of CO <sub>2</sub> and H <sub>2</sub> within the MOF materials.	<b>Resumo do projeto</b> O objetivo deste projeto é o desenvolvimento de materiais com grande potencial de adsorção/armazenamento de H <sub>2</sub> , CO <sub>2</sub> e outros gases baseados em estruturas metalorgânicas (do inglês, metal organic frameworks, MOFs) e covalentes (do inglês, covalent organic frameworks, COFs). Estes materiais funcionam como esponjas capazes de absorver, reter e liberar moléculas em seus poros. A principal inovação do projeto é usar Informática de Materiais combinando simulações moleculares multiescala, aprendizado de máquina e otimização de topologia para acelerar a seleção de triagem e projetar morfologias otimizadas para aumentar a seletividade de CO <sub>2</sub> e H <sub>2</sub> dentro os materiais MOF.

<b>Requirements for the candidate</b>	<b>Requisitos para o candidato</b>
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The candidate must have a PhD degree with experience in multiscale molecular simulations, machine learning, and topology optimization . English is required. The candidate must be interested in participating in a multidisciplinary project.

O candidato deve possuir doutorado e experiência em simulações moleculares multiescala, aprendizado de máquina e otimização topológica. Inglês é necessário. O candidato deve ter interesse em participar de projeto multidisciplinar.

#### NOTES

- This research scholarship is offered by the OTIC – Offshore Technology Innovation Centre, a research center based at the University of São Paulo, Brazil.
- The scholarship will cover a standard monthly stipend determined by the funding agencies.
- Foreign candidates must fulfill the immigration requirements and obtain the necessary visas to work as researchers in Brazil. (Help will be offered to the selected candidate.)
- After the application process, potential candidates will be invited for personal or remote interviews.

#### REQUIRED DOCUMENTS FOR APPLICATION

- Single-page presentation letter. Introduce yourself and share your motivations for applying for this position.
- Brief curriculum vitae with academic and professional experience, highlighting the skills that will contribute to this position.
- Recommendation letters (optional). One or two recommendation letters will help support your application.

#### APPLICATION PROCESS

- Prepare an e-mail to [otic.jobs@usp.br](mailto:otic.jobs@usp.br).
- Add “Application to [POSITION\_REF\_NUMBER]” to the subject.
- Gather all required documents above and attach them in PDF format.
- Send your application before the deadline above.

If you have any questions, please write to [otic.jobs@usp.br](mailto:otic.jobs@usp.br).