

Felipe LOPES DE OLIVEIRA

PhD student

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EDUCATION

Currently March 2020	Doctor in Science on Chemistry, UNIVERSIDADE FEDERAL DO RIO DE JANEIRO, UFRJ <ul style="list-style-type: none">> Fellowship : Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) 2020-2024> Supervisor : Prof. Pierre Mothé Esteves> Thesis : Atoms, Molecules and Frameworks : Exploring the interrelationships between molecular scales
March 2020 April 2018	Master of Science in Chemistry, UNIVERSIDADE FEDERAL DO RIO DE JANEIRO, UFRJ <ul style="list-style-type: none">> Fellowship : Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) 2018-2020> Supervisor : Prof. Pierre Mothé Esteves> Co-supervisor : Prof. Raoni Schroeder Borges Golçalves> Thesis : Study of new carbon allotropes by Density Functional Theory PDF
December 2017 April 2013	Bachelor in Nanoscience and Nanotechnology Bionanotechnology, UNIVERSIDADE FEDERAL DO RIO DE JANEIRO, UFRJ <ul style="list-style-type: none">> Fellowship : Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) 2015-2016> Fellowship : Monitor of Physics II 2017-2018> Undergraduate Research Project : Study of the application of paramagnetic ions as vanish mechanism in NMR experiments<ul style="list-style-type: none">- Supervisor : Prof. Marcius da Silva Almeida> Undergraduate Research Project : Covalent Organic Frameworks as a New Nanoporous Platform for the development of heterogeneous biocatalysis<ul style="list-style-type: none">- Supervisor : Prof. Raoni Schroeder Borges Golçalves

RESEARCH EXPERIENCE

Currently March 2021	Machine Learning application to accelerated materials discovery, INTERLAB-IQ, UFRJ <ul style="list-style-type: none">> Supervisor : Prof. Pierre Mothé Esteves
Currently March 2019	Physico-Chemical aspects of CO₂ capture by Covalent Organic Frameworks, INTERLAB-IQ, UFRJ <ul style="list-style-type: none">> Supervisor : Prof. Pierre Mothé Esteves> Paper highlighted as "Hot Paper" on the Chemistry - European Journal
Currently April 2018	Theoretical and Experimental study of new nanoporous carbon structures, INTERLAB-IQ, UFRJ <ul style="list-style-type: none">> Master thesis student> Supervisor : Prof. Pierre Mothé Esteves> Co-supervisor : Prof. Raoni Schroeder Borges Golçalves> Fellowship : Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq)> Paper added to the section "Hot Topic : Carbon, Graphite, and Graphene" of Wiley

December 2017	Covalent Organic Frameworks as a New Nanoporous Platform for the development of heterogeneous biocatalysis, LABORATORY OF CATALYSIS AND ORGANIC SYNTHESIS-IQ, UFRJ
November 2016	<ul style="list-style-type: none"> > Undergraduate internship > Supervisor : Prof. Raoni Schroeder Borges Golçalves > Paper highlighted as "Hot Paper" on the Chemistry - European Journal
September 2016	Study of the application of paramagnetic ions as vanish mechanism in NMR experiments, LABORATORY OF STRUCTURE-FUNCTION OF PROTEINS-CCS, UFRJ
November 2014	<ul style="list-style-type: none"> > Undergraduate internship > Supervisor : Prof. Marcius da Silva Almeida > Fellowship : Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq)

LANGUAGES

Portuguese ● ● ● ● ●
English ● ● ● ○ ○

QUANTUM-CHEMISTRY

Quantum ESPRESSO ● ● ● ● ○
Gaussian ● ● ● ○ ○
CP2K ● ● ● ○ ○
GAMESS ● ● ○ ○ ○
xTB ● ● ○ ○ ○
ORCA ● ● ● ○ ○
RASPA ● ● ● ● ○

HPC MANAGER

Slurm ● ● ● ● ○
PBS ● ● ● ○ ○

PROGRAMMING

Python ● ● ● ● ○
LaTeX ● ● ● ● ○
Bash ● ● ● ○ ○
TensorFlow ● ● ● ○ ○
scikit-learn ● ● ● ● ○
PyTorch ● ● ○ ○ ○

HONORS AND AWARDS

- 2019 Best Poster, 8° Congresso Brasileiro de carbono (CARBONO-2019).
2018 Best Poster Presentation, 17th Brazilian Meeting on Organic Synthesis (17th BMOS).

SUPERVISION OF UNDERGRADUATE STUDENT

Currently	João Matheus Souza Chagas, INTERLAB, URFJ
March 2021	<ul style="list-style-type: none"> > Project : Combining ML and DFT to accelerate the development of nanoporous materials
July 2021	Lucas Paodjuenas, INTERLAB, URFJ
January 2021	<ul style="list-style-type: none"> > Project : Addressing the influence of functional groups on the gas adsorption of nanoporous materials
July 2020	Júlia Nunes, INTERLAB, URFJ
July 2019	<ul style="list-style-type: none"> > Project : Comparative studies of gas adsorption on nanoporous materials
December 2019	Júlia Mina, INTERLAB, URFJ
March 2019	<ul style="list-style-type: none"> > Project : High surface area microporous materials from cigarette butt-derived waste
January 2020	Gabriel Vieira de Oliveira, INTERLAB, URFJ
June 2018	<ul style="list-style-type: none"> > Project : Tileynes : A family of 2D carbon allotropes

9. AN EXPERIMENTAL AND THEORETICAL STUDY OF HYDROXYLATED AZINE-BASED COVALENT ORGANIC FRAMEWORKS : INFLUENCE OF SURFACE AREA AND HETEROATOMS IN CO₂ CAPTURE

Renata Avena Maia, **Felipe Lopes Oliveira**, Vincent Ritleng, Qiang Wang, Benoît Louis, Pierre Mothé Esteves
Chemistry–A European Journal, Vol. 27, No. 30, p. 8048-8055, 2021

[DOI: 10.1002/chem.202100478](https://doi.org/10.1002/chem.202100478)

Covalent Organic Frameworks DFT CO₂ Capture Nanoporous Materials

8. FIRST-PRINCIPLES CALCULATIONS OF A NEW SEMI-CONDUCTIVE CARBON ALLOTROPE NAMED ABF-CARBON

Felipe L. Oliveira, Pierre M. Esteves
J. Braz. Chem. Soc. Vol. 32, No. 4, 869-877, 2021.

[DOI: 10.21577/0103-5053.20200238](https://doi.org/10.21577/0103-5053.20200238)

Carbon Allotrope DFT Semiconductive Carbon Nanoporous Carbons

7. A CARBOCATIONIC TRIARYLMETHANE-BASED COVALENT ORGANIC FRAMEWORK

Sunny de Freitas, **Felipe Lopes Oliveira**, Thigo Custódio dos Santos, Danilo Hisse, Claudia Merlini, Célia Machado Ronconi, Pierre Mothé Esteves

Chemistry–A European Journal, Vol. 27, No. 7, p. 2342-2347, 2021

[DOI: 10.1002/chem.202003554](https://doi.org/10.1002/chem.202003554)

Covalent Organic Networks DFT CO₂ Capture Microporous Materials

6. ENZYME IMMOBILIZATION IN COVALENT ORGANIC FRAMEWORKS : STRATEGIES AND APPLICATIONS IN BIOCATALYSIS

Felipe L. Oliveira, Alexandre de S. França, Aline Machado de Castro, Rodrigo O. M. Alves de Souza, Pierre M. Esteves, Raoni Schroeder B. Gonçalves

ChemPlusChem 85 (9), 2051-2066.

[DOI: 10.1002/cplu.202000549](https://doi.org/10.1002/cplu.202000549)

Biocatalysis Heterogeneous Catalysis Porous materials Nanostructures Enzymes Covalent Organic Frameworks

5. DYE-BASED COVALENT ORGANIC NANOSHEETS (CONS)

Sunny Freitas, **Felipe L Oliveira**, Claudia Merlini, Elizanne Justo, Adriana Gioda, Pierre M Esteves
JPhys Materials, 3(2) 025011

[DOI: 10.1088/2515-7639/ab854b](https://doi.org/10.1088/2515-7639/ab854b)

Covalent Organic Nanosheets DFT Organic Dyes Nanoporous Materials

4. Spiro-Carbon : A METALLIC CARBON ALLOTROPE PREDICTED FROM FIRST PRINCIPLES CALCULATIONS

Felipe L. Oliveira, Rodrigo B. Capaz, and Pierre M. Esteves.
ChemPhysChem, v. 21, n. 1, p. 59-64, 2020.

[DOI:10.1002/cphc.201900966](https://doi.org/10.1002/cphc.201900966)

Carbon Allotrope DFT Conductive Carbon Nanoporous Carbons

3. ENZYME-DECORATED COVALENT ORGANIC FRAMEWORK AS A NANOPOROUS PLATFORM FOR HETEROGENEOUS BIOCATALYSIS

Felipe L. Oliveira, Stefania P. de Souza, Jonathan Bassut, Heiddy M. Álvarez, Yunier Garcia-Basabe, Rodrigo O. M. Alves de Souza, Pierre M. Esteves, Raoni S. B. Gonçalves.

Chemistry–A European Journal, v. 25, n. 69, p. 15863-15870, 2019.

[DOI:10.1002/chem.201903807](https://doi.org/10.1002/chem.201903807)

Covalent Organic Framework Enzyme Biocatalysis Catalysis Enantiomeric Resolution Nanoporous Material

2. CRYSTAL ENGINEERING OF COVALENT ORGANIC FRAMEWORKS BASED ON HYDRAZINE AND HYDROXY-1, 3, 5-TRIFORMYLBENZENES

Renata A. Maia, **Felipe L. Oliveira**, Michael Nazarkovsky, and Pierre M. Esteves.

Crystal Growth & Design 18, no. 9 (2018) : 5682-5689.

[DOI:10.1021/acs.cgd.8b01110](https://doi.org/10.1021/acs.cgd.8b01110)

Covalent Organic Frameworks Crystallinity Conformational Locks Modulator

1. N-DIAMONDYNES : EXPANDING THE FAMILY OF CARBON ALLOTROPES

Deyse G. Costa, Fábio JFS Henrique, **Felipe L. Oliveira**, Rodrigo B. Capaz, and Pierre M. Esteves
Carbon 136 (2018) : 337-344

[DOI:10.1016/j.carbon.2018.04.073](https://doi.org/10.1016/j.carbon.2018.04.073)

Carbon Allotrope DFT Porous Carbons Diamondynes