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
- 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
- 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
- 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
  - Supervisor : Prof. Marcius da Silva Almeida
- Undergraduate Research Project : Covalent Organic Frameworks as a New Nanoporous Platform for the development of heterogeneous biocatalysis
  - Supervisor : Prof. Raoni Schroeder Borges Golçalves

Research Experience

Currently – March 2021 | Machine Learning application to acelerated materials discovery, Interlab-IQ, UFRJ
- Supervisor : Prof. Pierre Mothé Esteves

Currently – March 2019 | Physico-Chemical aspects of CO_2 capture by Covalet Organic Frameworks, Interlab-IQ, UFRJ
- 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
- 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 – November 2016

Covalent Organic Frameworks as a New Nanoporous Platform for the development of heterogeneous biocatalysis, Laboratory of Catalysis and Organic Synthesis-IQ, UFRJ

- Undergraduate intership
- Supervisor : Prof. Raoni Schroeder Borges Golçalves
- Paper highlighted as "Hot Paper" on the Chemistry - European Journal

September 2016 – November 2014

Study of the application of paramagnetic ions as vanish mechanism in NMR experiments, Laboratory of Structure-Function of Proteins-CCS, UFRJ

- Undergraduate intership
- Supervisor : Prof. Marcius da Silva Almeida
- Fellowship : Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq)

HPC softwares

Slurm	●●●●○
PBS	●●●○○

Languages

Portuguese	●●●●●
English	●●●○○

Quantum-Chemistry

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

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 – March 2021

João Matheus Souza Chagas, Interlab, URFJ

- Project : Combining ML and DFT to accelerate the development of nanoporous materials

July 2021 – January 2021

Lucas Paodjuenas, Interlab, URFJ

- Project : Addressing the influence of functional groups on the gas adsorption of nanoporous materials

July 2020 – July 2019

Júlia Nunes, Interlab, URFJ

- Project : Comparative studyes of gas adsorption on nanoporous materials

December 2019 – March 2019

Júlia Mina, Interlab, URFJ

- Project : High surface area microporous materials from cigarette butt-derived waste

January 2020 – June 2018

Gabriel Vieira de Oliveira, Interlab, URFJ

- Project : Tileynes : A family of 2D carbon allotropes

Publications

9. An Experimental and Theoretical Study of Hydroxylated Azine-Based Covalent Organic Frameworks : Influence of Surface Area and Heteroatoms in CO_2 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

Covalent Organic Frameworks | DFT | CO_2 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

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

Covalent Organic Networks | DFT | CO_2 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

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

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

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

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

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

Carbon Allotrope | DFT | Porous Carbons | Diamondynes