Curriculum
M.Sc. Johnatan Mucelini

1 Personal Information

Name: Johnatam Mucelini

Currently: **PhD Student** in the QTNano Lab

Advisor: Juarez L. F. Da Silva.

Affiliation: São Carlos Institute of Chemistry (IQSC)
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2 Education

1. **PhD** in Physical Chemistry (2018-Present-2022)
   - University of São Paulo (USP), São Carlos Institute of Chemistry, São Carlos, Brazil.
   - Advisor: Juarez L. F. Da Silva.
   - Keywords: Atomistic Simulation, Data Mining, and Machine Learning.
   - Scientific Production: two article (2nd and 3rd author) (see they in the next section).
   - Grade: A (maximun) in all courses.
2. **MSc** in Physical Chemistry (2016-2018).
   - University of São Paulo (USP), São Carlos Institute of Chemistry, São Carlos, Brazil.
   - Advisor: Juarez L. F. Da Silva.
   - Master thesis (in Portuguese): link to the repository.
   - Keywords: Atomistic Simulation, CeO2, Desity functional Theory.
   - Scientific Production: one 1st author article and a 2nd author book chapter (see it in the next section)
   - Grade: A (maximun) in all courses.
3. **BSc** in Chemistry (2013-2016)
   - Ferderal University of Santa Cataina, Department of Chemistry, Florianópolis, Brasil.

- Advisor: Giovanni F. Caramori.
- Undergraduate thesis (in Portuguese): link to the repository.
- Keywords: Cation-π interaction, π-π interaction, Transition metal complexes.
- Scientific Production: one 1st author article (see it in the next section).
- Grade Point Average: 8.54/10.

3 Scientific Production

1. Article (**2nd** author): Methane dehydrogenation on 3*d* 13-atom transition-metal clusters: A density functional theory investigation combined with Spearman rank correlation analysis. Fuel, **2020**, 275, 117790. DOI: 10.1016/j.fuel.2020.117790
2. Article (**3rd** author): *Ab Initio* Insights Into the Formation Mechanisms of 55-Atom Pt-c ased Core-Shell Nanoalloys. The Journal of Physical Chemistry, **2020**, 124, 1, 1158-1164. DOI: 10.1021/acs.jpcc.9b09561
3. Article (**2nd** author): *Ab initio* insights into the structural, energetic, electronic, and stability properties of mixed $Ce_nZr_{15-n}O_{30}$ nanoclusters, Physical Chemistry Chemical Physics, **2019**, 21, 26637-26646. DOI: 10.1039/C9CP04762J
4. Article (**1st** author): *Ab initio* investigation of the formation of ZrO_2-like structures upon the adsorption of Zr_n on the CeO_2(111) surface, The Journal of Chemical Physics, **2018**, 149, 244702. DOI: 10.1063/1.5063732
5. Article (**1st** author): Understanding the interplay between π-π and cation-π interactions in [janusene-Ag]$^+$ host-guest systems: a computational approach, Dalton Transactions, **2019**, 48, 13281-13292. DOI: 10.1039/C9DT02307K
6. Book chapter (**2nd** author): From Bulk CeO_2 to Transition-Metal Clusters Supported on the CeO_2(111) Surface: A Critical Discussion. In book: **Encyclopedia of Interfacial Chemistry, Surface Science and Electrochemistry**, 2018, 452-459. DOI: 10.1016/B978-0-12-409547-2.14196-4

4 Provided Hands-ons and Talks

1. Hands-on (3 days) entitled "**Machine Learning Aplications and Introdution to Data Analysis with Python**", in the IV CINE-CMSC Workshop: Machine Learning Techniques Applied to Computational Material Science with Hands-on, which occurred in São Carlos, São Paulo, from February 10 to 14, 2020.

2. Open talk entitled "**A Correlation and Feature Engineering Based Framework to Obtain Insights from Quantum Chemistry Datasets**" in the IV CINE-CMSC Workshop: Machine Learning Techniques Applied to Computational Material Science with Hands-on, which occurred in São Carlos, São Paulo, from February 10 to 14, 2020.

3. Open talk entitled "**Data Mining and Statistical Tools based Framework to Investigate Quantum Chemistry Data**" in the III CINE-CMSC Workshop, which occurred in São Carlos, São Paulo, from September 02 to 06, 2019.

4. Hands-on (3 days) entitled "**Tutorial on Vienna Ab initio Simulation Package (VASP)**", in the II CINE-CMSC Workshop, which occurred in São Carlos, São Paulo, from February 13 to 15, 2019.

5. Open talk entitled "**Ab initio on investigation of Zr Adatoms on the CeO_2(111) surface**" in the III School of Computational Chemistry, which occurred in Ribeirão Preto, São Paulo, from December 11 to 14, 2017.

5 Research Grants Awarded

1. 2018-2022: National Council for Scientific and Technological Development (CNPq) **PhD's degree fellowship**.

2. 2016-2018: CNPq **master's degree fellowship**.

6 Ongoing Researches

- I am **developing a Data Mining framework** (**python implementation**) that allows the user to deeply analyze the relationship between the atomic environment and some property of interest, such as the cohesive energy (related to stability) and the band bag (important optical property). An important point of this methodology is that it describes the atomic systems in terms of physical meaningful features. This work was employed in three papers until now (10.1021/acs.jpcc.9b09561, 10.1039/C9CP04762J, and 10.1021/acs.jpcc.9b09561). Right now, we are writing a paper that will address this methodology in more detail.

- I am **collaborating with two Machine Learning (ML) experts** (Prof. Dr. Ronaldo C. Prati and Prof. Dr. Marcos G. Quiles) in two projects related to applications of ML algorithms in quantum chemistry datasets: "Machine learning prediction of nine molecular properties based on the SMILES representation of the QM9 dataset" and "Quantifying the bias-variance decomposition in materials science data set".

- I am **co-supervising the Undergraduate Student in Chemistry Mariana Candido Gallego** (Supervised by Prof. Dr. Juarez Lopes Ferreira Da Silva in the São Carlos Institute of Chemistry - University of São Paulo) in her scientific initiation program. She is performing an investigation of the structural, energetic, and optical properties of ABX_3 perovskites for solar cell applications, employ first-principles calculations.