

Israel C. Ribeiro

Ph.D in Physical–Chemistry | Computational Materials Science

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🎓 Google Scholar

🐙 GitHub

in linkedin.com/in/israel-ribeiro1

Academic Background

Ph.D in Theoretical Physical Chemistry

University of São Paulo (USP)

📅 November 2020 – November 2025 📍 São Carlos, Brazil

- Research Thesis: Atomic-scale Investigations into the Metallic and Organic Passivation of Two-Dimensional Perovskite Thin Films
- Advisor: Professor Juarez L. F. Da Silva

MBA in Data Science and Analytics

University of São Paulo (USP)

📅 October 2024 – August 2026 📍 Online, Distance Learning

- Final Project: Machine Learning Applied to Material Science
- Advisor: Professor Viviane Ferreira

BSc in Chemistry, minored in Chemistry of Materials

Federal University of São Joao del Rei (UFSJ)

📅 March 2015 – November 2020 📍 São João del Rei, Brazil

- Undergraduate Research Thesis: Theoretical Investigation of Structural and Electronic Properties of GaN in the Haeckelita 8-4 Structure
- Advisor: Professor Horacio W. Alvez

Research Experience

University of São Paulo

Ph.D Candidate

📅 2020 – 2025 📍 São Carlos, Brazil

- Experience with plane-wave-based first-principles simulations for structural and optoelectronic properties;
- Strong background in computational materials design, high-throughput screening, data-driven modeling, and optimization of materials for specific properties, using multi-scale simulations;
- Skilled in data wrangling, visualization, statistical analysis, and automation with Python and related tools for large-scale dataset handling and post-processing.

Federal University of São João del Rei

Undergraduate Research

📅 2015 – 2020 📍 São João del Rei, Brazil

- Experience in sol-gel synthesis of inorganic nanomaterials, with a focus on doping rare earth-based materials;
- Knowledge of characterization techniques, including XRD, TGA, FTIR, UV-Vis spectroscopy, spectrofluorimetry, BET surface area analysis, and SEM/TEM for structural, thermal, optical, and morphological analysis;
- Experience with first-principles simulations to study electronic structure and molecular interactions.

Areas of Interest

- Materials Science;
- Density Functional Theory;
- Data Science and Analytics;
- Inorganic Materials;
- Quantum Chemistry.

Teaching Assistant

General Chemistry II

University of São Paulo (USP)

📅 August 2023 – December 2023

📍 São Carlos, Brazil

Inorganic Chemistry II

University of São Paulo (USP)

📅 October 2020 – January 2023

📍 São Carlos, Brazil

Fundamentals of Quantum Chemistry

Natural Sciences Department (UFSJ)

📅 March 2019 – July 2019

📍 São João del Rei, Brazil

Chemistry of Materials

Natural Sciences Department (UFSJ)

📅 March 2018 – July 2018

📍 São João del Rei, Brazil

Article Reviewer

- Journal of Molecular Physics

Languages

Portuguese ●●●●●

English ●●●●●

French ●●●●●

Industry Experience

AMG Brazil

Chemical Process Intern

📅 2015 – 2018

📍 São João del Rei, Brazil

- Conducted fluoride and chloride analysis, as well as elemental analysis using ICP;
- Conducted quality control and performance tests, ensuring product compliance with industry regulations and improving reliability;
- Executed process optimization tests and prepared detailed technical reports;
- Led the implementation of the 5S program, improving laboratory efficiency and organization.

Resind LTDA

Chemical Technician

📅 2019 – 2020

📍 São João del Rei, Brazil

- Oversaw quality tests for primary products, ensuring compliance with standards;
- Conducted quantitative chemical analyses using X-ray techniques;
- Maintained product excellence and reliability through comprehensive assessments.

Scientific Publications

Impact of Thin Film Thickness on the Structural, Energetic and Optoelectronic Properties of Two-Dimensional $\text{FPEA}_2(\text{MA}_{n-1})\text{Pb}_n\text{I}_{3n+1}$ Perovskites

ACS Applied Energy Materials

📅 2025

DOI: 10.1021/acsaem.4c02800

Authors: **Israel C. Ribeiro**, Felipe D. Picoli, Pedro Ivo R. Moraes, André F. V. Fonseca, Luiz N. Oliveira, Ana Flávia Nogueira and Juarez L. F. Da Silva.

Unveiling the Impact of Organic Cation Passivation on Structural and Optoelectronic Properties of Two-Dimensional Perovskites Thin Films

Applied Surface Science

📅 2024

DOI: 10.1016/j.apsusc.2024.161098

Authors: **Israel C. Ribeiro**, Pedro Ivo R. Moraes, Albert F. B. Bittencourt and Juarez L. F. Da Silva.

Role of the Adsorption of Alkali Cations on Ultrathin n -Layers of Two-Dimensional Perovskites

Journal of Physical Chemistry C

📅 2023

DOI: 10.1021/acs.jpcc.3c01894

Authors: **Israel C. Ribeiro**, Pedro Ivo R. Moraes, Albert F. B. Bittencourt and Juarez L. F. Da Silva.

Academic Schools

CNPEM-IBM School Sustainable Materials & AI

📅 April 2025

📍 Campinas, Brazil

Metal Halides Perovskites for Optoelectronic: from Fundamental to Devices

📅 October 2024

📍 Roscoff, France

São Paulo School of Advanced Science on Quantum Materials

📅 July 2024

📍 São Paulo, Brazil

XVIII Brazilian School of Electronic Structure

📅 October 2023

📍 Campinas, Brazil

Highlights Talks

The Chemistry Beyond Haber–Bosch Process

PechaKucha Seminar IFSC–USP

📅 May 2024

📍 São Carlos, Brazil

Overview on the Adsorption and Surface Properties of Perovskite-based Materials for Solar Cell Applications

X Center for Innovation on New Energies (CINE) Workshop

📅 June 2023

📍 São Carlos, Brazil

Energy Transfer from Tb^{3+} to Eu^{3+} Inside of the Matrix $\text{SiO}_2\text{-TiO}_2$

18th International Conference on Luminescence

📅 August 2017

📍 João Pessoa, Brazil

CaTiO₃:Er³⁺:Yb³⁺ Upconversion from 980 nm to 1550 nm
Excitation and its Potential as Cells Luminescent Probes

Materials Chemistry and Physics

📅 2019

DOI: 10.1016/j.matchemphys.2018.11.018

Authors: Rafael Perrella, **Israel C. Ribeiro**, Paulo Campos-Junior, Marco Schiavon, Pecoraro, and Jefferson Ferrari.

Delving into Transition Metal Single-atom Doping Effects in
Two-Dimensional Perovskite Thin Films

Status: Pending Submission

📅 2025

Authors: **Israel C. Ribeiro**, Lucas G. Chagas, Jilian N. de Freitas,
Matheus P. Lima and Juarez L. F. Da Silva.

Enhanced Catalytic Efficiency in Ammonia Synthesis:
The Role of Ferrites and Graphenes in Electrocatalytic
Reduction of N₂

Status: Pending Submission

📅 2025

Authors: Clécia Andrade dos Santos, Marina Medina da Silva, Lariel
Chagas da Silva Neres, **Israel C. Ribeiro**, Horácio W. Alves, Luciane
Pimenta Cruz Romão and Maria V. Boldrin Zanoni.

Role of Ni, Cu, Ag, and Au Points Defects in the
Degradation of MAPbI₃ Perovskite

Status: Pending Submission

📅 2025

Authors: Lucas G. Chagas, **Israel C. Ribeiro**, Jilian N. de Freitas,
Matheus P. Lima and Juarez L. F. Da Silva.

Ab initio Investigation on Structural and Electronic
Properties of 2D III-Nitride Monolayers

Status: Pending Submission

📅 2025

Authors: **Israel C. Ribeiro** and Horácio W. Alves.

Phenylphosphonic Acid-Induced Surface Passivation in
MAPbI₃ Perovskite Thin Films

Status: Calculations Running

📅 2025

Authors: **Israel C. Ribeiro**, Iván Ornelas-Cruz, Matheus P. Lima and
Juarez L. F. Da Silva.

Unraveling the Origins of Exciton Binding Energies in
Two-Dimensional Ga₂O₃, Ag₂Se₂ and SnI₂ Compounds

Status: Calculations Running

📅 2025

Authors: Felipe D. Picoli, Gustavo Diniz, **Israel C. Ribeiro**, Luiz N.
Oliveira and Juarez L. F. Da Silva.

Chemistry Software

VASP ● ● ● ● ●

Quantum Espresso ● ● ● ● ●

FHI-aims ● ● ● ● ●

Gaussian ● ● ● ● ●

Programming

Python ● ● ● ● ●

R ● ● ● ● ●

Julia ● ● ● ● ●

Tools & Technologies

SQL ● ● ● ● ●

TensorFlow ● ● ● ● ●

Scikit-Learn ● ● ● ● ●

Power BI ● ● ● ● ●

Letters of Recommendation

• Prof. Luiz Nunes de Oliveira (USP)
✉ luizno@usp.br

• Prof. Marcelo Henrique Gehlen (USP)
✉ marcelog@iqsc.usp.br

• Prof. Horacio W. Alvez (UFSJ)
✉ hwlalves@ufs.edu.br

• Prof. Jefferson L. Ferrari (UFU)
✉ jeffersonferrari@ufu.br