Rafael R. Del Grande | Merced, CA, USA | rafaeldgrande@gmail.com | +1(209)-308-2022
Personal Page | Google Scholar (93 citations, h-index=4)| GitHub | Linkedin

Researcher with a PhD in condensed matter physics and deep experience in computational materials science, high-performance computing, and scientific software development in both academic and industry settings. Skilled in first-principles simulations (DFT, GWBSE), molecular dynamics, data analysis/automation using python and bash. Experienced in HPC clusters (SLURM/CPU/GPU), and currently transitioning into machine learning with a focus on AI-driven materials research. Passionate about applying and developing computational tools to solve real-world problems in nanotechnology, energy, and material science.

EXPERIENCE

University of California, Merced | Postdoctoral Scholar | Merced, CA, USA | **Jul 2021 - Current**

- Developed a program that calculates excited-state forces, integrating electron-phonon coupling with excitonic effects
- Automated and optimized the workflow of excited state forces calculations that combines DFPT and GWBSE results
- Performed relaxation of excited states in materials, including polaronic excitons in LiF, structural changes in 2D transition metal dichalcogenides, and perovskites
- Prediction of GW corrections using Neural Networks
- Construction of graph neural network force fields trained with excited state forces

Federal University of Rio de Janeiro | Research and Teaching Assistant | Rio de Janeiro, RJ, Brazil | **Mar 2015 - Jun 2021**

- Investigated self-trapped excitons in carbon nanotubes with sp^3 defects
- Used genetic algorithm to fit tight binding parameters to perform electronic structure calculations of carbon nanotubes with random distributions of defects
- Performed DFT simulations and classical force field relaxations of twisted multi-layer graphene

Federal University of Rio de Janeiro | Lecturer | |Rio de Janeiro, RJ, Brazil | **Aug 2018 - Jul 2020**

- Taught undergraduate physics (theory and experimental labs)
- Adapted experimental classes to a remote format during COVID-19 pandemic

IBM | Research Intern | Rio de Janeiro, RJ, Brazil | **Dec 2013 - Mar 2015 and Oct 2015 – May 2016**

- Studied wettability at nanoscale for Enhanced Oil Recovery
- Performed classical molecular dynamics simulations of nano drops to be compared with experimental results
- Developed coarse-grained models towards bigger classical molecular dynamics simulations

F**ederal University of Rio de Janeiro** | Scientific Initiation Student |Rio de Janeiro, RJ, Brazil| **Oct 2011 - Feb 2015**

- Performed molecular dynamics simulations of the local collapse of carbon nanotubes

SKILLS

Programming & Data Analysis: Python (NumPy, SciPy, Matplotlib, Jupyter Notebooks, ASE), Bash, Mathematica
Software Development & Tools: Git, Scrum, Docker, GenAI tools (ChatGPT, Copilot), Latex, HTML
Machine Learning: TensorFlow, PyTorch
Computational Methods: High Performance Computing (SLURM, CPUs & GPUs), Tight Binding, Molecular Dynamics (LAMMPS), Density Functional Theory (Quantum Espresso), Many Body Perturbation Theory (BerkeleyGW), Wannier functions (Wannier90).
Languages: Portuguese (Native), English (Fluent), Spanish (Intermediate), French (Basic)

EDUCATION

Ph.D. in Physics Federal University of Rio de Janeiro | Rio de Janeiro, Brazil | Mar 2017 - Jun 2021
Thesis title: Consequences of H Doping in the Electronic and Optical Properties of Carbon Nanotubes
Awarded *Bolsa nota 10* - excellence fellowship from FAPERJ (Rio de Janeiro state funding agency) | Apr 2020 - Jun 2021
M.Sc. in Physics Federal University of Rio de Janeiro | Rio de Janeiro, Brazil | Mar 2015 - Feb 2017
Thesis title: Influence of van der Waals corrections on multi-layer graphene/graphite systems in Density Functional Theory
B.Sc. in Nanoscience and Nanotechnology Federal University of Rio de Janeiro | Rio de Janeiro, Brazil | Mar 2011 - Feb 2015

Selected Additional Courses / Workshops

- (2025) Deep Learning Specialization. DeepLearning.AI on Coursera.
- (2025) Machine Learning Specialization. Stanford University & DeepLearning.AI on Coursera.
- (2024) Machine Learning Summer Institute. Texas Advance Computing Center, University of Texas, Austin.
- (2022) School on Electron-Phonon Physics from First Principles. University of Texas, Austin.
- (2022) 9th Time-dependent Density Functional Theory: Prospects and Applications. Benasque, Spain.
- (2021) Excited States and Nonadiabatic Dynamics CyberTraining Workshop. University at Buffalo. Online