INIFTA

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Universidad Zagoza

1474

Horizon 2020:
Marie Curie Research and Innovation Staff Exchange

Santiago D. Barrionuevo

MELON

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Horizon 2020:
Marie Curie Research and Innovation Staff Exchange

Visiting dates: September 2022 (Ph.D. student) & September 2024 (Postdoc)

Activities:

•Worked **synthesis and characterization** of two-dimensional (2D) materials aimed at nanoelectronics applications.

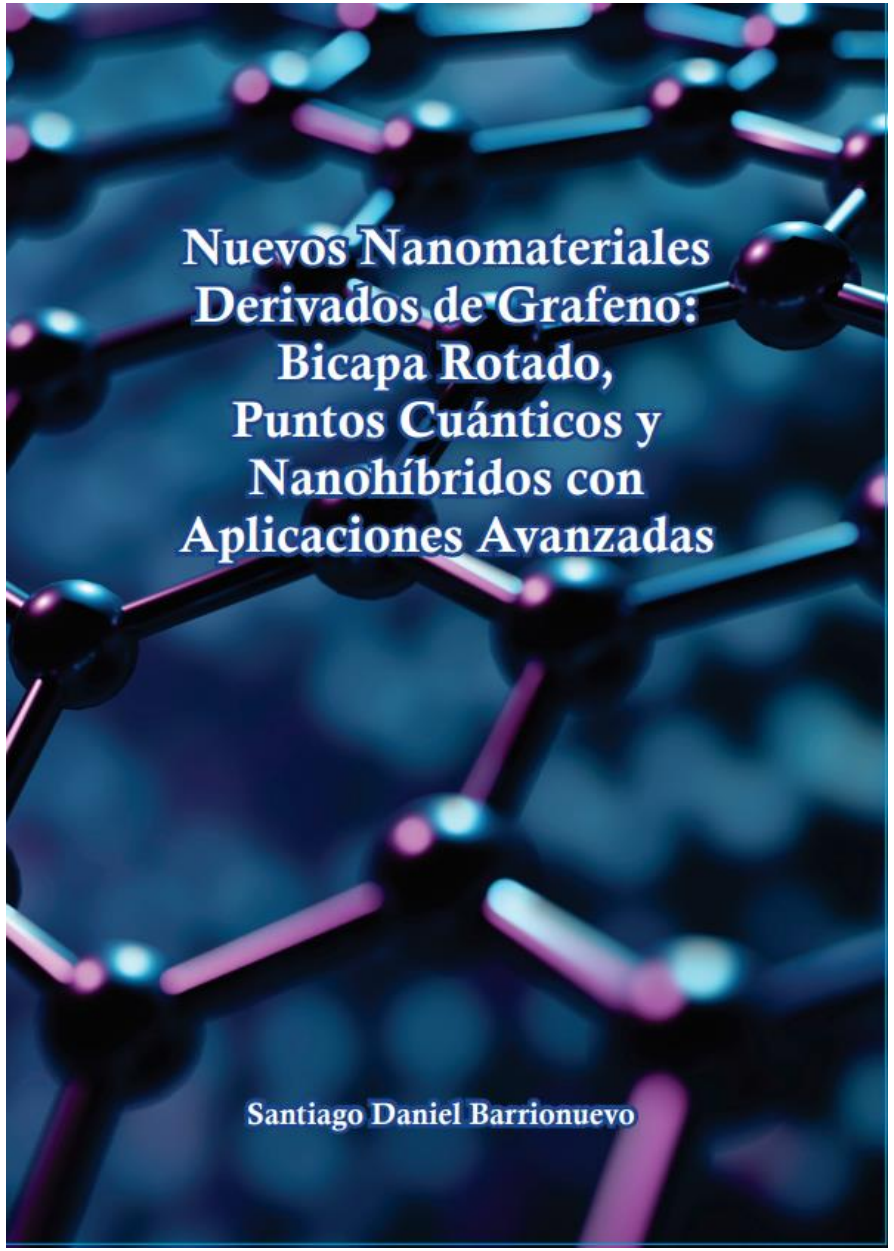
•Developed several synthesis and transfer techniques for **graphene and graphene-derived nanomaterials.**

•Worked on the advanced characterization of these nanomaterials using high-resolution transmission electron microscopy (**HRTEM**), scanning transmission electron microscopy (**STEM**), energy-dispersive X-ray spectroscopy (**EDS**), and electron energy-loss spectroscopy (**EELS**).

MELON

Santiago D. Barrionuevo

Published Thesis



Published Work (4)

1. **Barrionuevo, S. D.**; Fioravanti, F.; Nuñez, J. M.; Muñeton Arboleda, D.; Lacconi, G. I.; Bellino, M. G.; Aguirre, M. H.; Ibañez, F. J. Stacking-Configuration-Preserved Graphene Quantum Dots Electrochemically Obtained from CVD Graphene. *J. Phys. Chem. C* **2024**, *128* (3), 1393–1403. https://doi.org/10.1021/acs.jpcc.3c06871.

2. **Barrionuevo, S. D.**; Fioravanti, F.; Nuñez, J. M.; Llaver, M.; Aguirre, M. H.; Bellino, M. G.; Lacconi, G. I.; Ibañez, F. J. Efficient Generation of Highly Crystalline Carbon Quantum Dots via Electrooxidation of Ethanol for Rapid Photodegradation of Organic Dyes. *J. Mater. Chem. C* **2023**, *11* (34), 11719–11729. https://doi.org/10.1039/D3TC01774E.

3. Llaver, M.; **Barrionuevo, S. D.**; Nuñez, J. M. M.; Chapana, A.; Wuilloud, R. G.; Aguirre, M. H.; Ibañez, F. J. Fluorescent Graphene Quantum Dots-Enhanced Machine Learning for Accurate Detection and Quantification of Hg2+ and Fe3+ in Real Water Samples. Environ. Sci.: Nano **2024**. https://doi.org/10.1039/D3EN00702B.

4. **Barrionuevo, S. D.** New Nanomaterials derived from Graphene: Twisted Bilayer Graphene, Graphene Quantum Dots and Graphene-Metal Nanohybrids with Advanced Applications. Thesis PhD Engineering. SEDICI. 2024. https://doi.org/10.35537/10915/169400

Submitted/Drafted Work (3)

1. **Barrionuevo, S. D.***; Ventre, J*.; Nuñez, J. M.; Renna, A.; Aguirre, M. H.; Bellino, M. G.; Ibañez, F. J. GQDs toward the Spontaneous Synthesis of core-shell Au-graphene Nanohybrid for Non-enzymatic Glucose Detection. ACS Applied Nanomaterials **2025** (Submitted) *** Both First Authors**

2. **Barrionuevo, S. D.**; Nuñez, J. M.; Ibañez, F. J. ; M. Aguirre. Size Threshold for Edge State Emergence in Graphene Quantum Dots (GQDs). **2025** Manuscript.

3. **Barrionuevo, S. D.**; Nuñez, J. M.; Ibañez, F. J. ; M. Aguirre. Synthesis and Characterization of Twisted Bilayer Graphene via Wet Transfer & HRTEM/EELS. **2025** Manuscript.

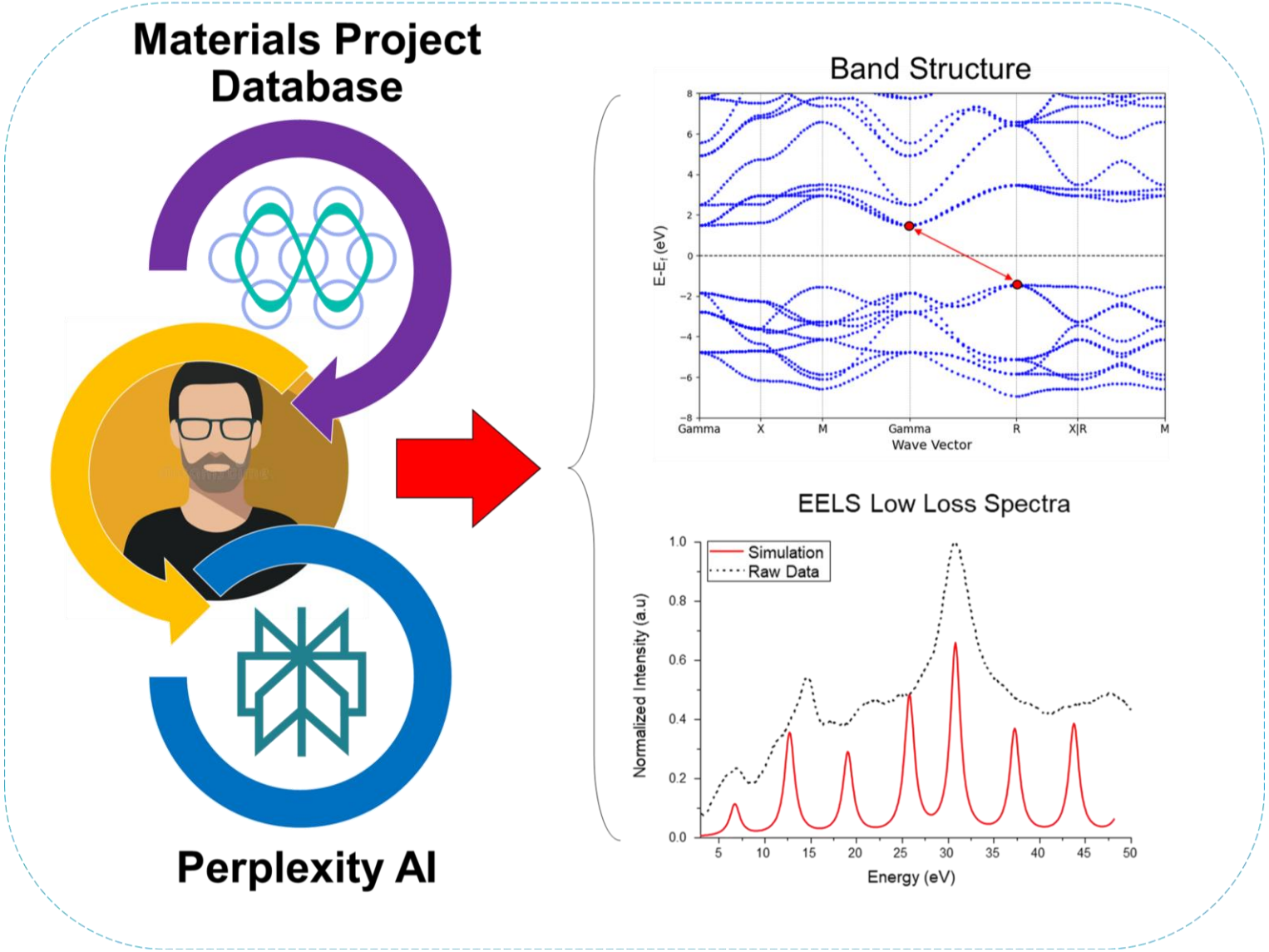
Awarded Proposals (2)

1. **Barrionuevo, S. D.**; M. Aguirre. Size Threshold for Edge State Emergence in Graphene Quantum Dots (GQDs). ELECMI 2024/**2025** Awarded Proposal.

2. **Barrionuevo, S. D.**; M. Aguirre. Electronic Structure Analysis of Twisted Bilayer Graphene at Specific Rotation Angles. ELECMI 2024/**2025** Awarded Proposal.

Current Work

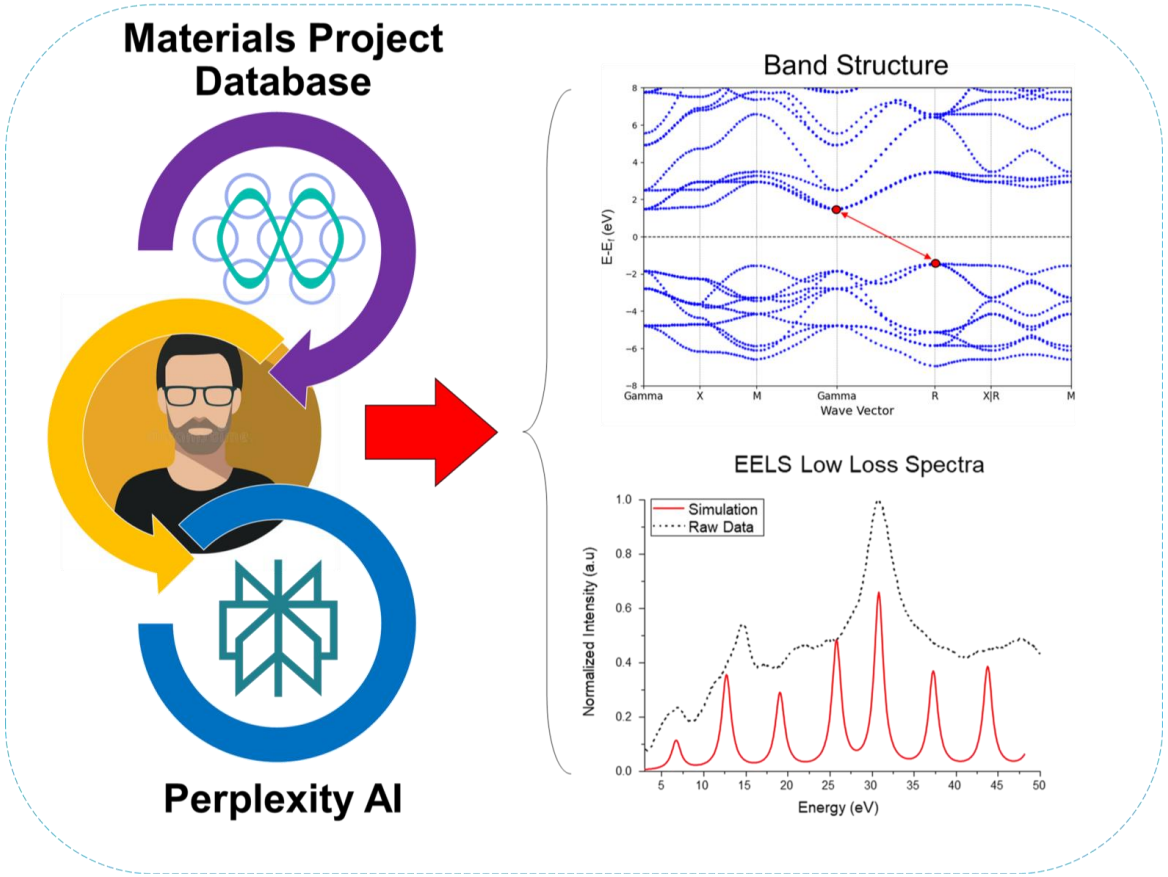
Developing an AI assisted Neuromorphic Material Simulator

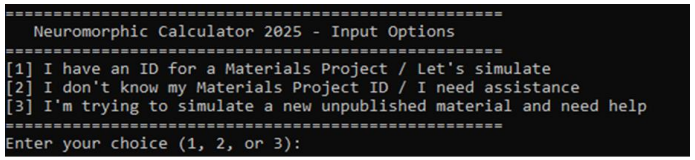


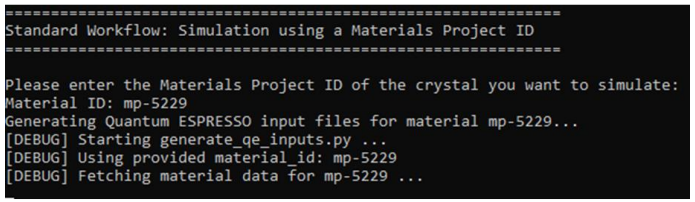
Current Work

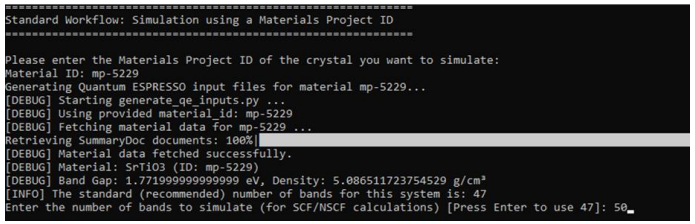
Developing an AI assisted Neuromorphic Material Simulator

Summary:
The Neuromorphic Calculator 2025 is a robust simulation platform that streamlines the process of performing first-principles materials calculations with Quantum ESPRESSO.









Current Work

Developing an AI assisted Neuromorphic Material Simulator

Summary:
The Neuromorphic Calculator 2025 is a robust simulation platform that streamlines the process of performing first-principles materials calculations with Quantum ESPRESSO.

It has three modes of operation tailored to different user needs.

In the **Standard Mode** mode, if you already have a Materials Project ID, you can quickly simulate that material's properties.

In the **AI Assistant Mode**, if you don't have a specific ID, the AI will help you find suitable materials based on your initial data and requirements. Then, it will set up the simulation and run it for you.!

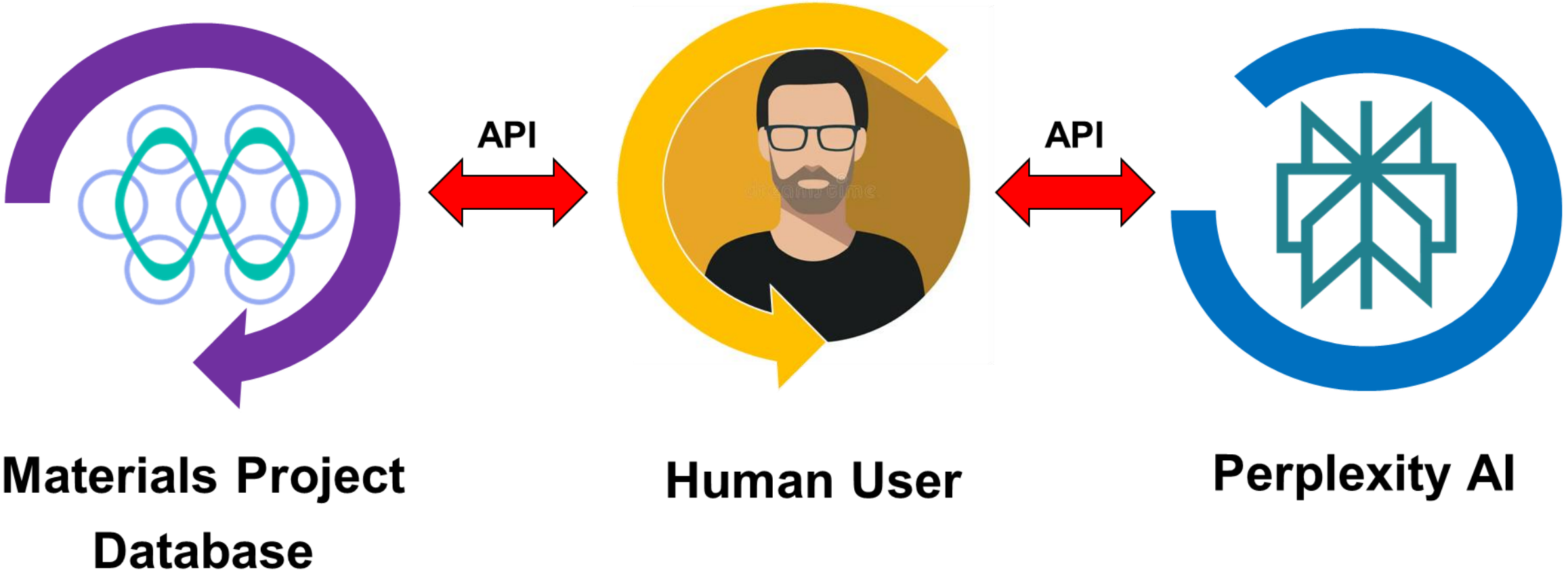
And in the **AI Expert Mode** it will help you think about new or unpublished materials, allowing you to customize parameters and refine them over multiple runs. It will ask you to be more involved in the design of each simulation and its going to address , correct and tailor the calculation in order to be consistent with the current literature of the topic you choose e.g.: Neuromorphic, Topological or Superconductor materials. The limit is on you!

Across all three modes, **AI is fully integrated**, generating input files, optimizing simulation parameters, providing literature-backed suggestions, and pulling the latest references for your work.
All of this is accomplished using top-tier AI models from Perplexity AI and the Materials Project Database, in order to provide new tools for AI-driven research.

Current Work

Developing an AI assisted Neuromorphic Material Simulator

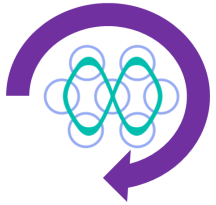
- **How does it work?**



Current Work

Developing an AI assisted Neuromorphic Material Simulator

- **How does it work?**



Materials Project Database

Human User

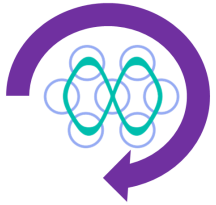
Perplexity AI

- **What can you do?**
  - **SCF (Self-Consistent Field) Calculation :** Determines the ground-state electronic structure of your system.
  - **NSCF (Non-Self-Consistent Field) Calculation:** Uses a fixed charge density from an SCF calculation to obtain eigenvalues and wavefunctions on a finer k-point grid.
  - **BANDS Calculation:** Calculate eigenvalues along a high-symmetry path in reciprocal space to analyze electronic band dispersion.
  - **DOS (Density of States) Calculation:** Computes the distribution of electronic states as a function of energy, often requiring a denser k-point sampling.
  - **EELS (Electron Energy Loss Spectroscopy) Calculation**: Simulates the energy loss spectrum of electrons interacting with the material, revealing information about plasmons and core-loss edges.

Current Work

Developing an AI assisted Neuromorphic Material Simulator

- **How does it work?**



Materials Project Database

Human User

Perplexity AI

- **What can yo do?**

•SCF (Self-Consistent Field)

•NSCF (Non-Self-Consistent Field)

•BANDS Calculation

•DOS (Density of States)

•EELS (Electron Energy Loss Spectroscopy)

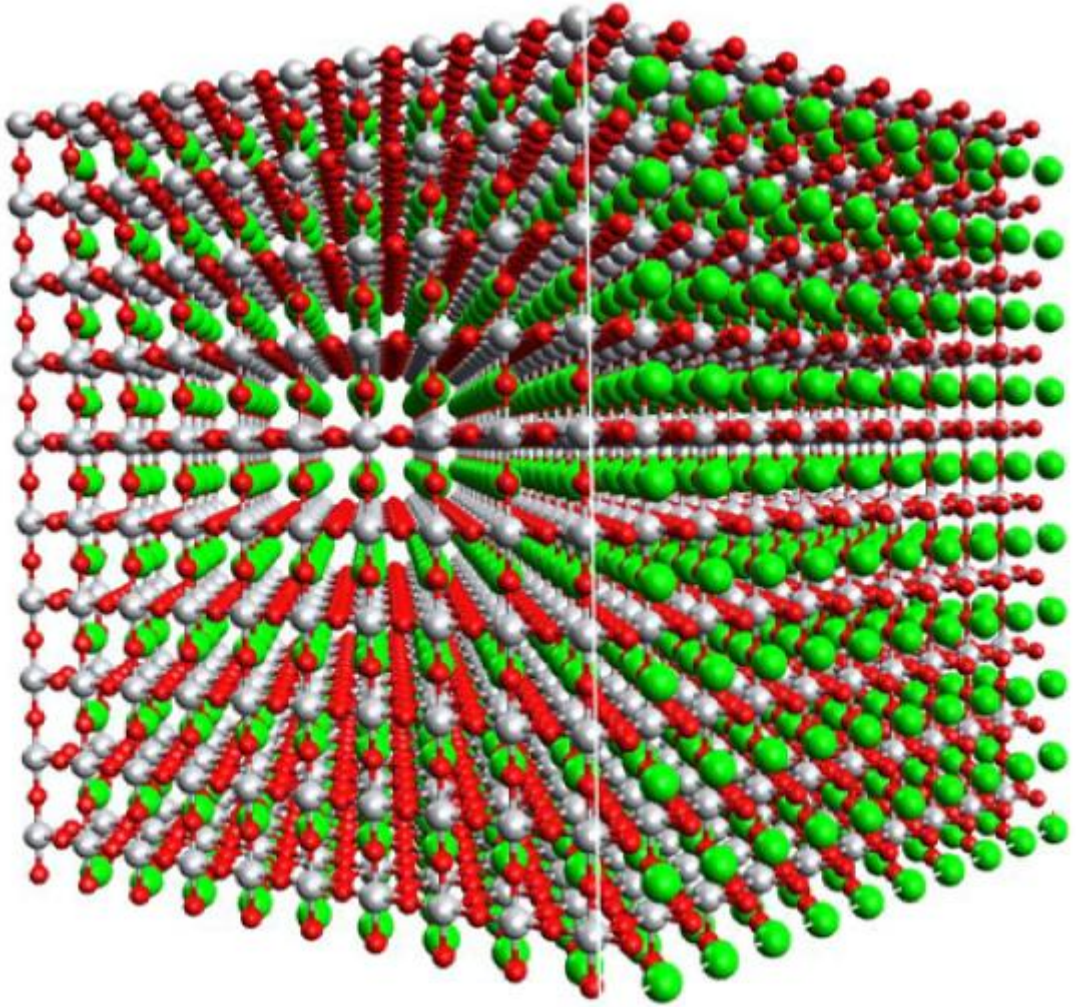
- **Where can I find it?**

https://github.com/SantiagoBLP/NeuroCalc2025_1.0

Current Work

Developing an AI assisted Neuromorphic Material Simulator:

Example Case SrTiO3 (Cubic)



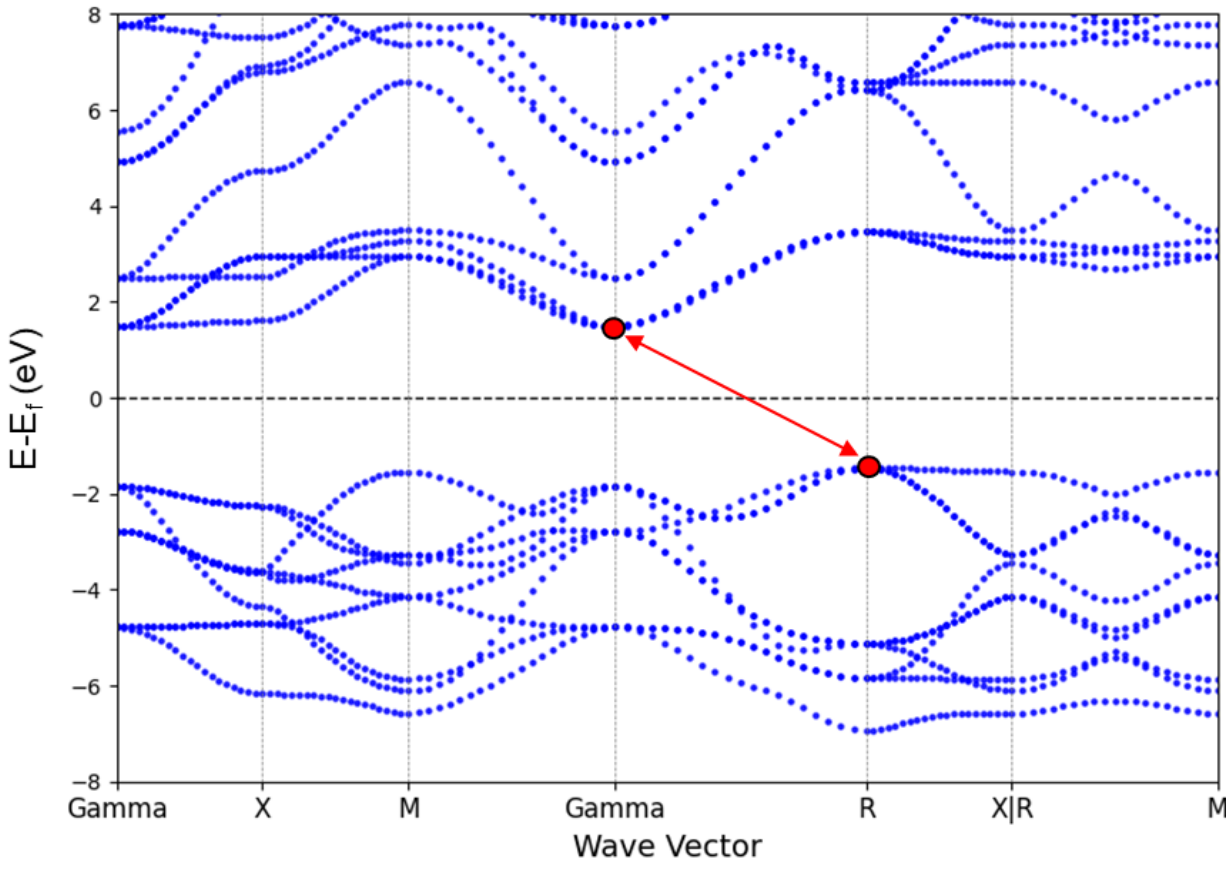
Sr2+ Ti4+ O2-

Current Work

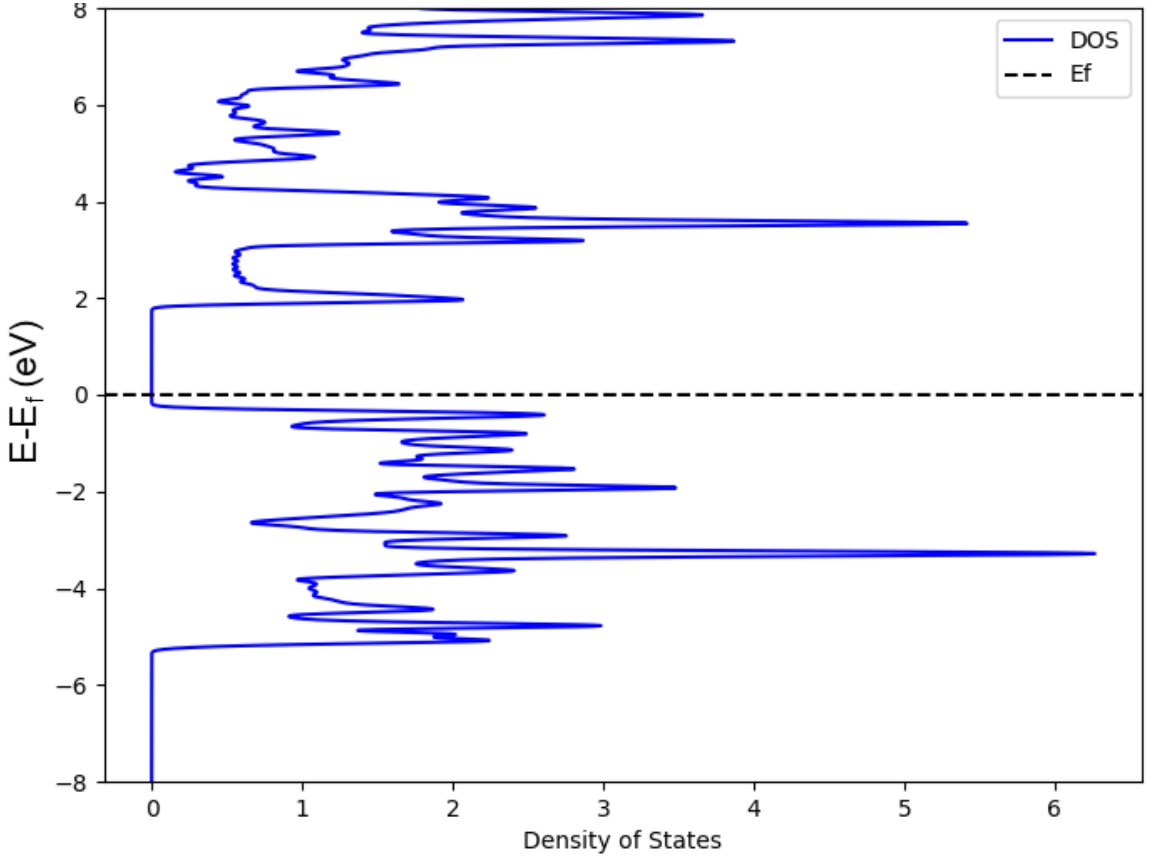
Developing an AI assisted Neuromorphic Material Simulator:

Example Case SrTiO3 (Cubic)

Band Structure



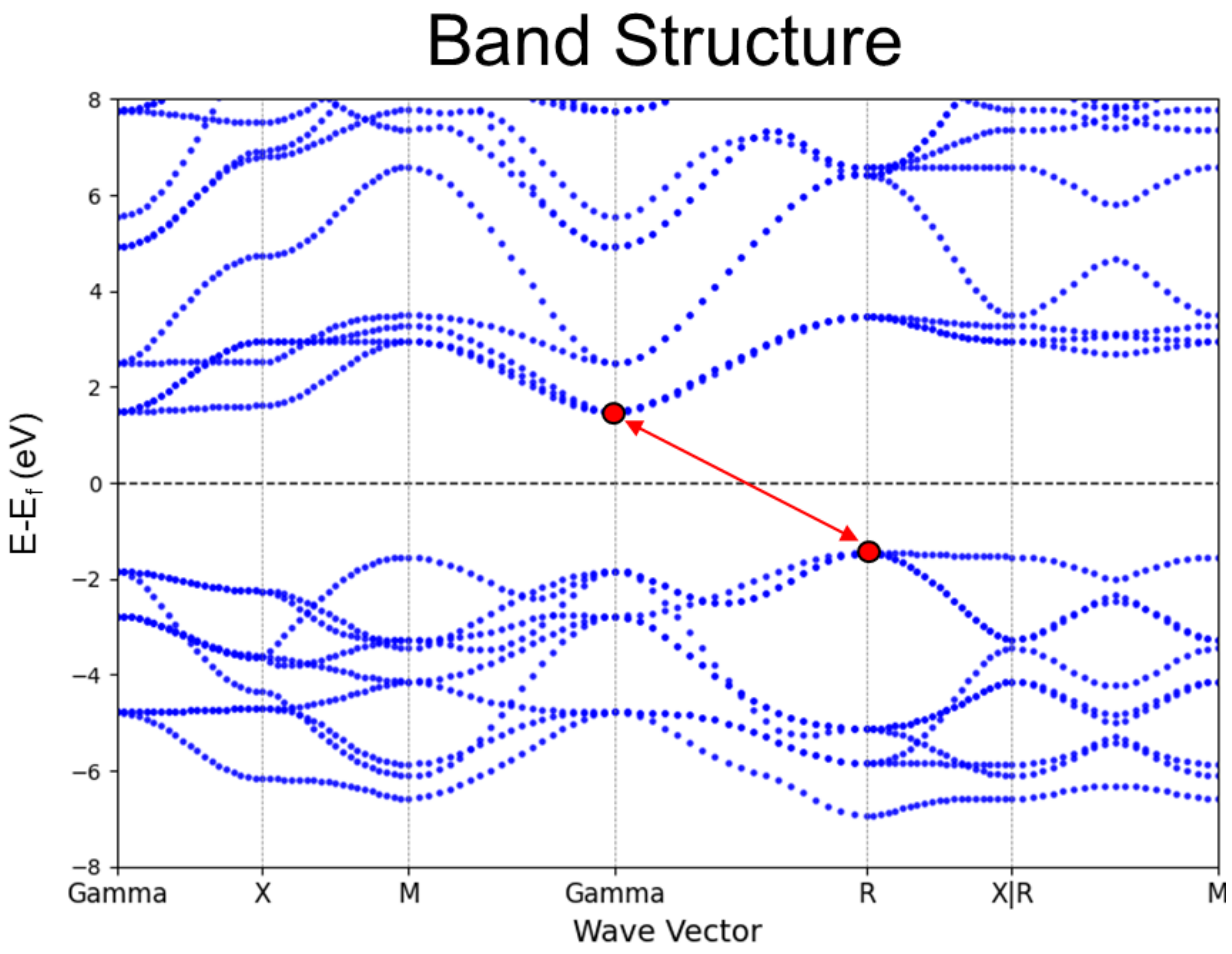
Density of State (DOS)

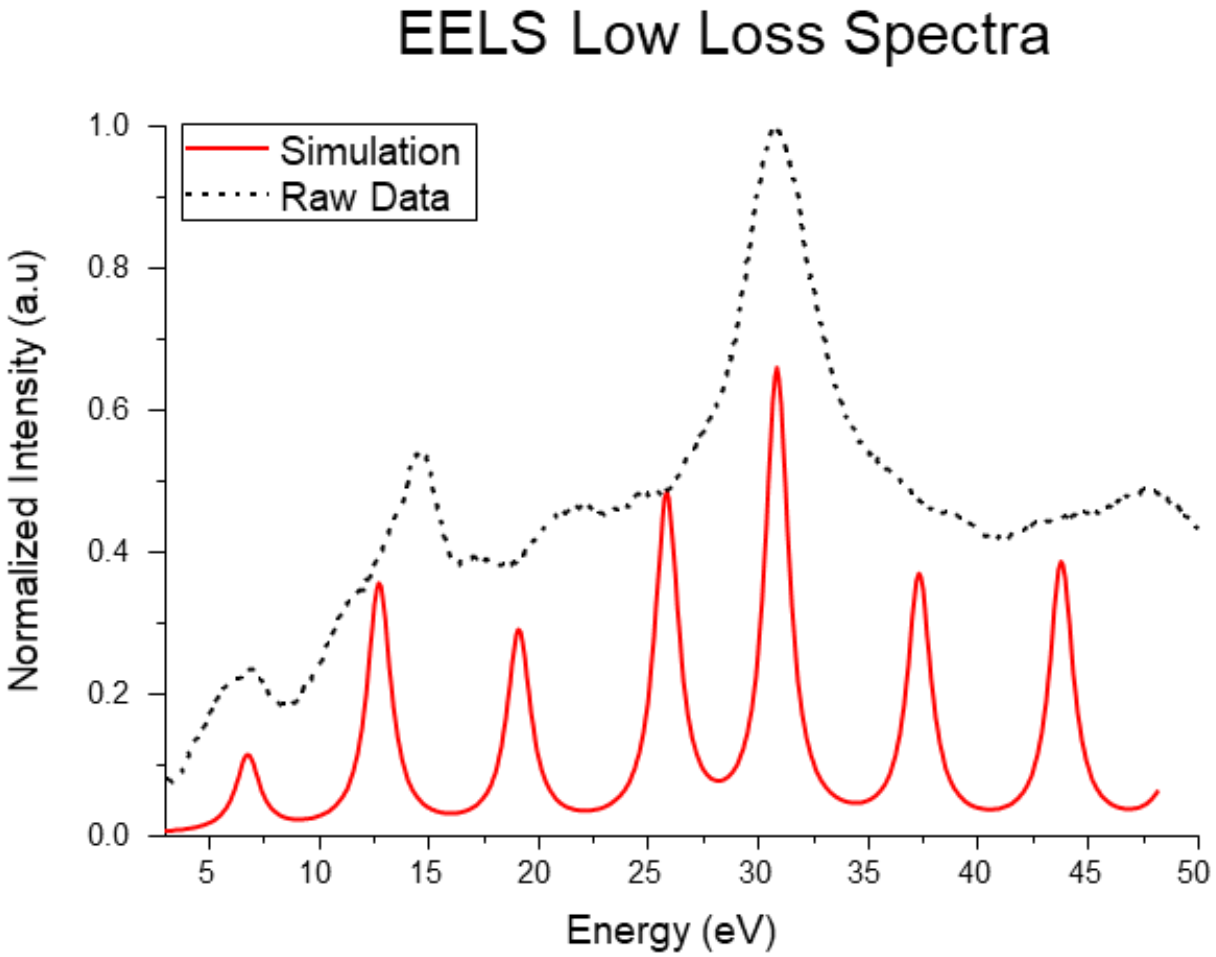


Current Work

Developing an AI assisted Neuromorphic Material Simulator:

Example Case SrTiO3 (Cubic)






Thank You!
santi.barri@unizar.es