

# Horizon 2020: Marie Curie Research and Innovation Staff Exchange

Santiago D. Barrionuevo



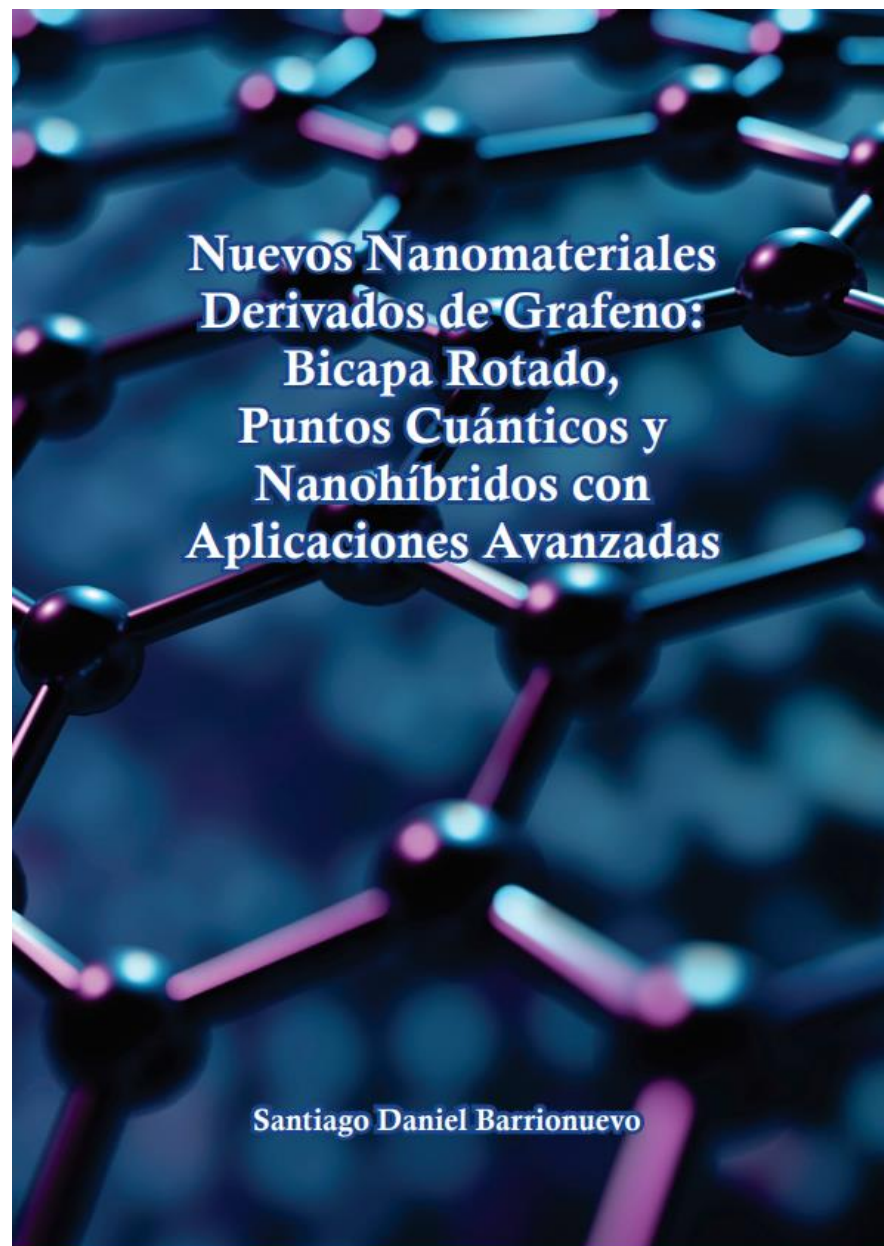
# Horizon 2020: Marie Curie Research and Innovation Staff Exchange

**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**).

## 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 Hg<sup>2+</sup> and Fe<sup>3+</sup> 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)

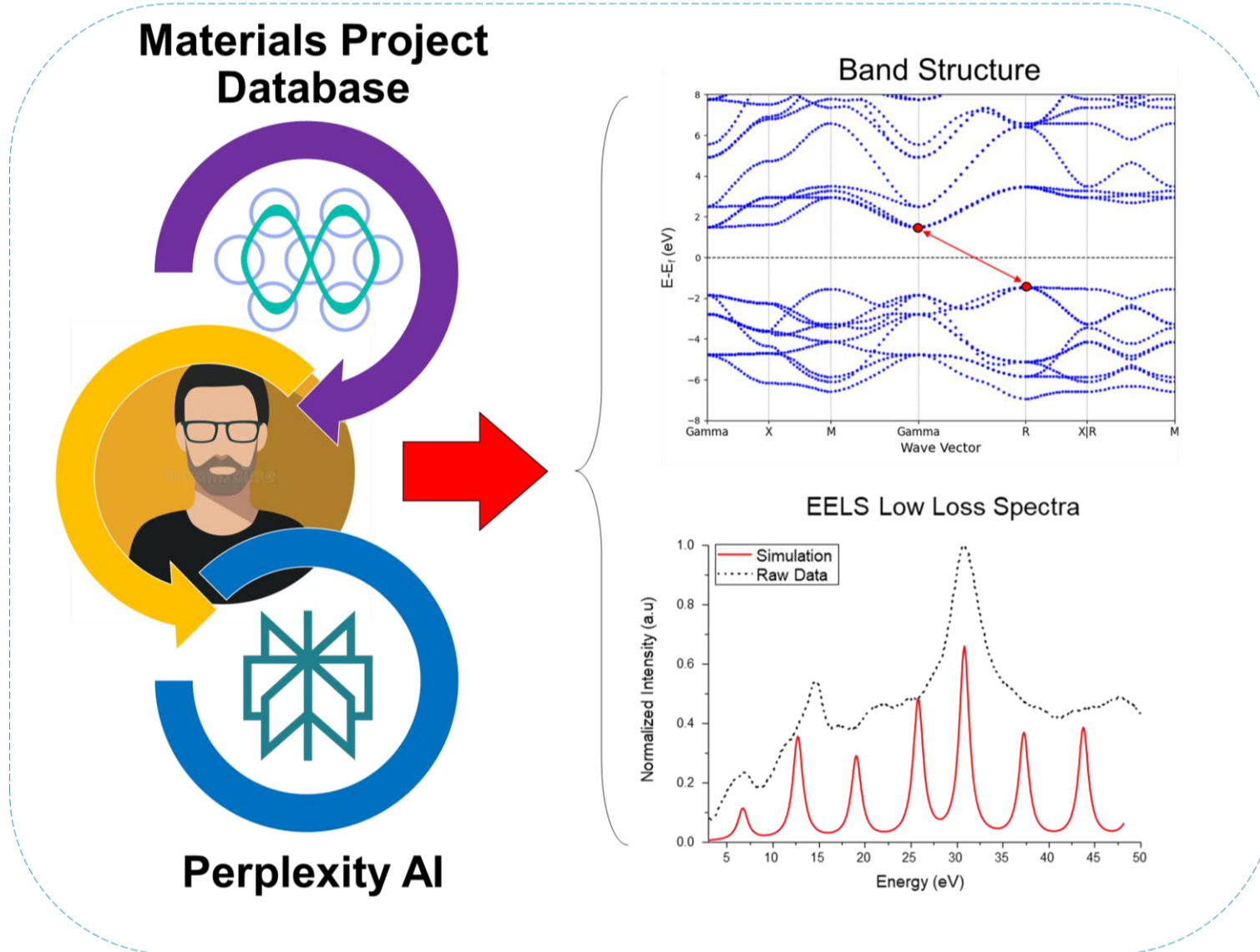
1. **Barrionuevo, S. D.\***; Ventre, J\*.; Nuñez, J. M.; Renna, A.; Aguirre, M. H.; Bellino, M. G.; Ibañez, F. J. GQDs toward the Spontaneous Synthesis of core-shell Au-graphene Nanohybrid for Non-enzymatic Glucose Detection. *ACS Applied Nanomaterials* **2025** (Submitted) \* **Both First Authors**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





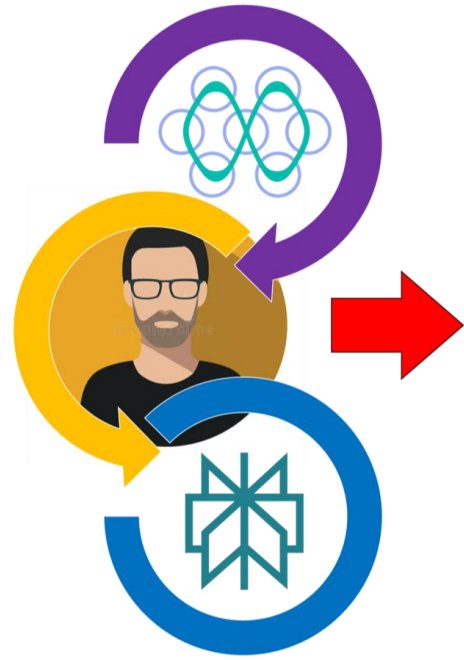
# Current Work

## Developing an AI assisted Neuromorphic Material Simulator

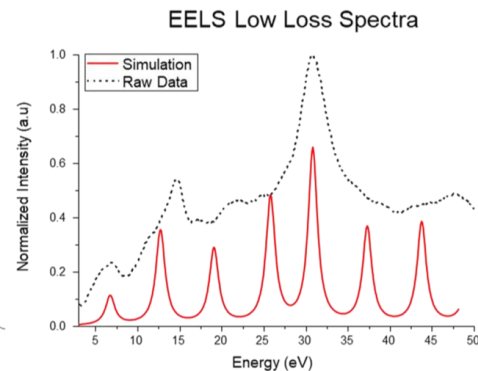
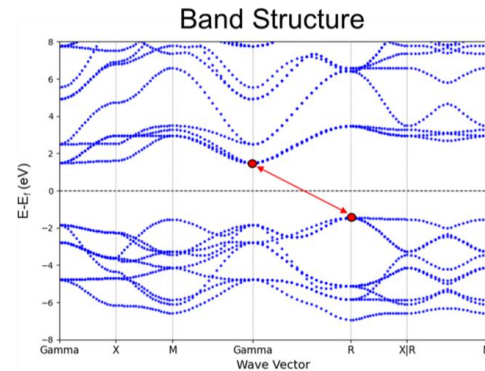
### Summary:

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

### Materials Project Database



### Perplexity AI



```
=====
WELCOME to the Neuromorphic Materials Calculator 2025!
=====
Developed by Dr. Ing. Santiago D. Barrionuevo
Under the supervision of Dra. Myriam H. Aguirre
=====
This project is funded by the EU project MELON as part of
HORIZON-2020 Marie Curie Research and Innovation Staff Exchange Action
Empowering students and researchers with first-principles tools
for simulating materials in neuromorphic applications (and more..!).
=====
Neuristive and multiferroic materials for logic units in nanoelectronics
=====

MELON MISSION
The most simplistic computational model of a neuron is an 'on-off' switch,
with a '0' representing a resting state and a '1' representing an axon firing
an action potential. While this lends itself well to conventional digital
electronics and silicon-based transistors, it does not represent the incredible
natural 'state' space of a real neuron. When it comes to realising the potential
of a brain-like processing system, novel materials are needed.
The EU-funded MELON project has created an expert consortium of academic
institutions and an SME to explore novel materials with history-dependent
conductivity to emulate neuronal connectivity. Together with materials capable
of multivalued logic and interconnects, the team plans to deliver the building
blocks of tomorrow's emergent computing circuits.

This program is crucial in simulating the materials that compose the heart
of these neuromorphic devices, helping researchers explore their electronic
and spintronic properties through first-principles calculations.
=====

How it works:
- Simulation & AI Assistance for Material Science:
Leverage our tool to simulate material properties and assist your research projects.

- Literature Review:
Our AI searches relevant literature to support your project with up-to-date
information and proper citations without hallucinations.

- Multiple Modes:
(1) Existing Materials:
If you already know the material you want to simulate
simply enter its Materials Project ID.
(2) Exploring Options:
If you're uncertain about the ID or are exploring potential materials
use our AI engine to find the ideal candidate.
(3) Pushing the Frontier of Science:
For experts creating new materials or pushing research boundaries
our AI assists in designing your ideal candidate.

- Seamless Workflow:
The program automatically handles the following:
- AI search engine and assistance to the user.
- Generation of Quantum ESPRESSO input files.
- Execution of SCF, NSCF, bands, DOS, and EELS calculations.
- Processing and visualization of the resulting data.

- Future Enhancements:
Stay tuned-more functionalities are coming soon!
=====

[ Press ENTER or SPACE to continue ]
```

```
=====
Neuromorphic Calculator 2025 - Input Options
=====
[1] I have an ID for a Materials Project / Let's simulate
[2] I don't know my Materials Project ID / I need assistance
[3] I'm trying to simulate a new unpublished material and need help
=====
Enter your choice (1, 2, or 3):

=====
Standard Workflow: Simulation using a Materials Project ID
=====

Please enter the Materials Project ID of the crystal you want to simulate:
Material ID: mp-5229
Generating Quantum ESPRESSO input files for material mp-5229...
[DEBUG] Starting generate_qe_inputs.py ...
[DEBUG] Using provided material_id: mp-5229
[DEBUG] Fetching material data for mp-5229 ...

=====
Standard Workflow: Simulation using a Materials Project ID
=====

Please enter the Materials Project ID of the crystal you want to simulate:
Material ID: mp-5229
Generating Quantum ESPRESSO input files for material mp-5229...
[DEBUG] Starting generate_qe_inputs.py ...
[DEBUG] Using provided material_id: mp-5229
[DEBUG] Fetching material data for mp-5229 ...
Retrieving SummaryDoc documents: 100%
[DEBUG] Material data fetched successfully.
[DEBUG] Material: SrTiO3 (ID: mp-5229)
[DEBUG] Band Gap: 1.7719999999999999 eV, Density: 5.086511723754529 g/cm³
[INFO] The standard (recommended) number of bands for this system is: 47
Enter the number of bands to simulate (for SCF/NSCF calculations) [Press Enter to use 47]: 50
```

# 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!

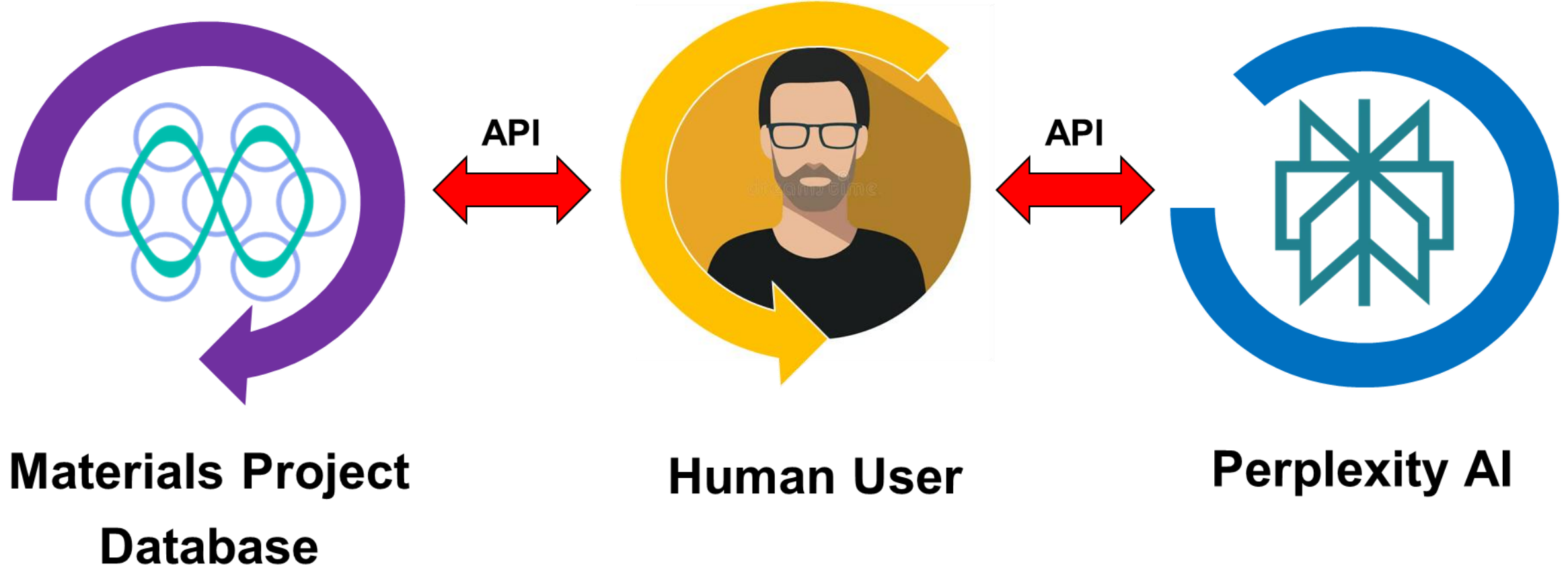
Across all three modes, **AI is fully integrated**, generating input files, optimizing simulation parameters, providing literature-backed suggestions, and pulling the latest references for your work.

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

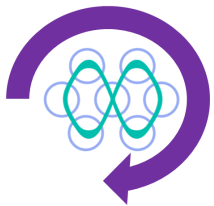
- How does it work?



# Current Work

## Developing an AI assisted Neuromorphic Material Simulator

- How does it work?



Materials Project  
Database



Human User



Perplexity AI

- What can you do?

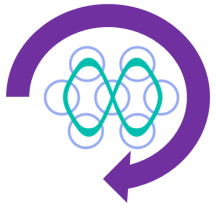
- **SCF (Self-Consistent Field) Calculation** : Determines the ground-state electronic structure of your system.
- **NSCF (Non-Self-Consistent Field) Calculation**: Uses a fixed charge density from an SCF calculation to obtain eigenvalues and wavefunctions on a finer k-point grid.
- **BANDS Calculation**: 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?

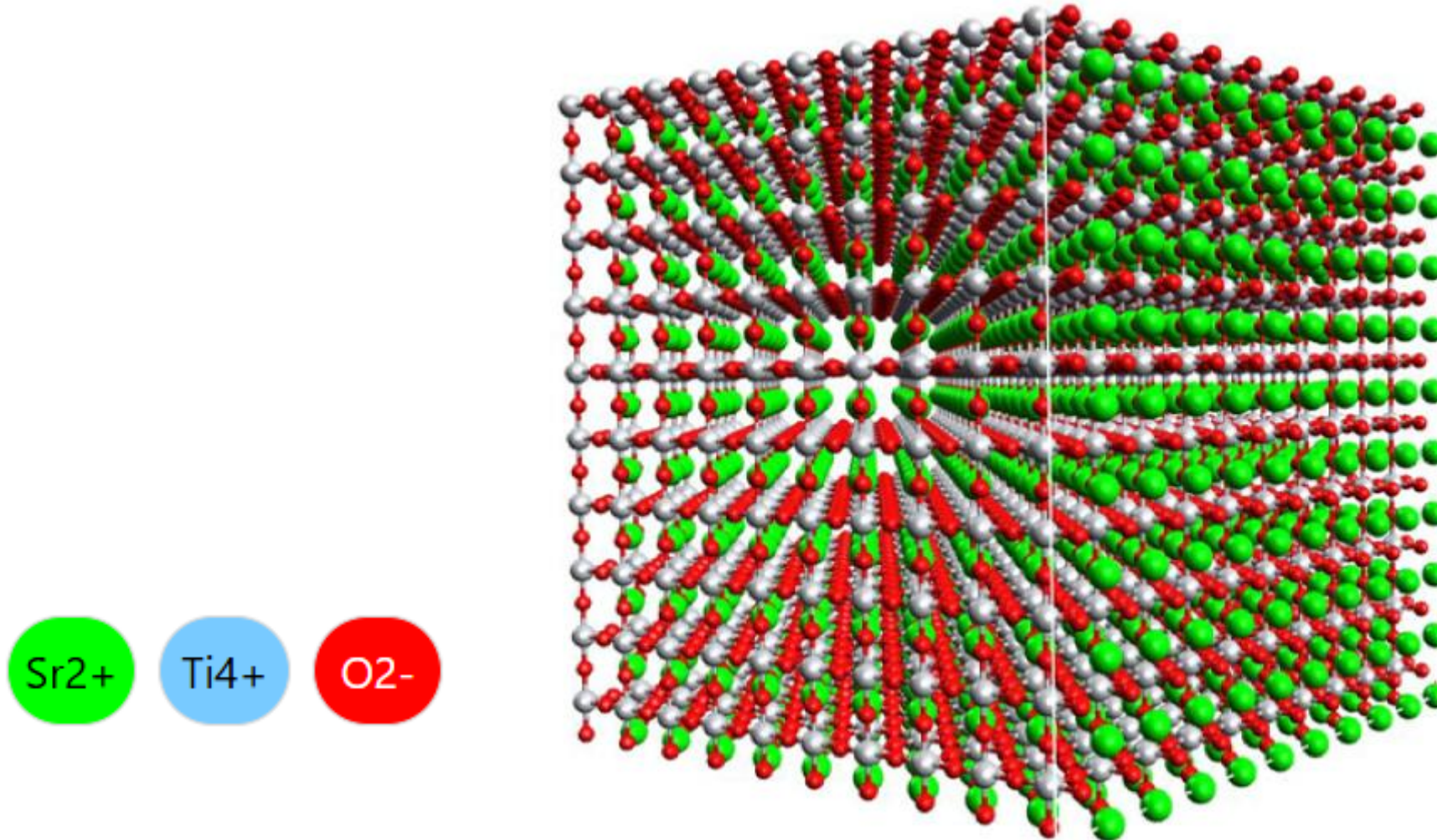


[https://github.com/SantiagoBLP/NeuroCalc2025\\_1.0](https://github.com/SantiagoBLP/NeuroCalc2025_1.0)

# Current Work

Developing an AI assisted Neuromorphic Material Simulator:

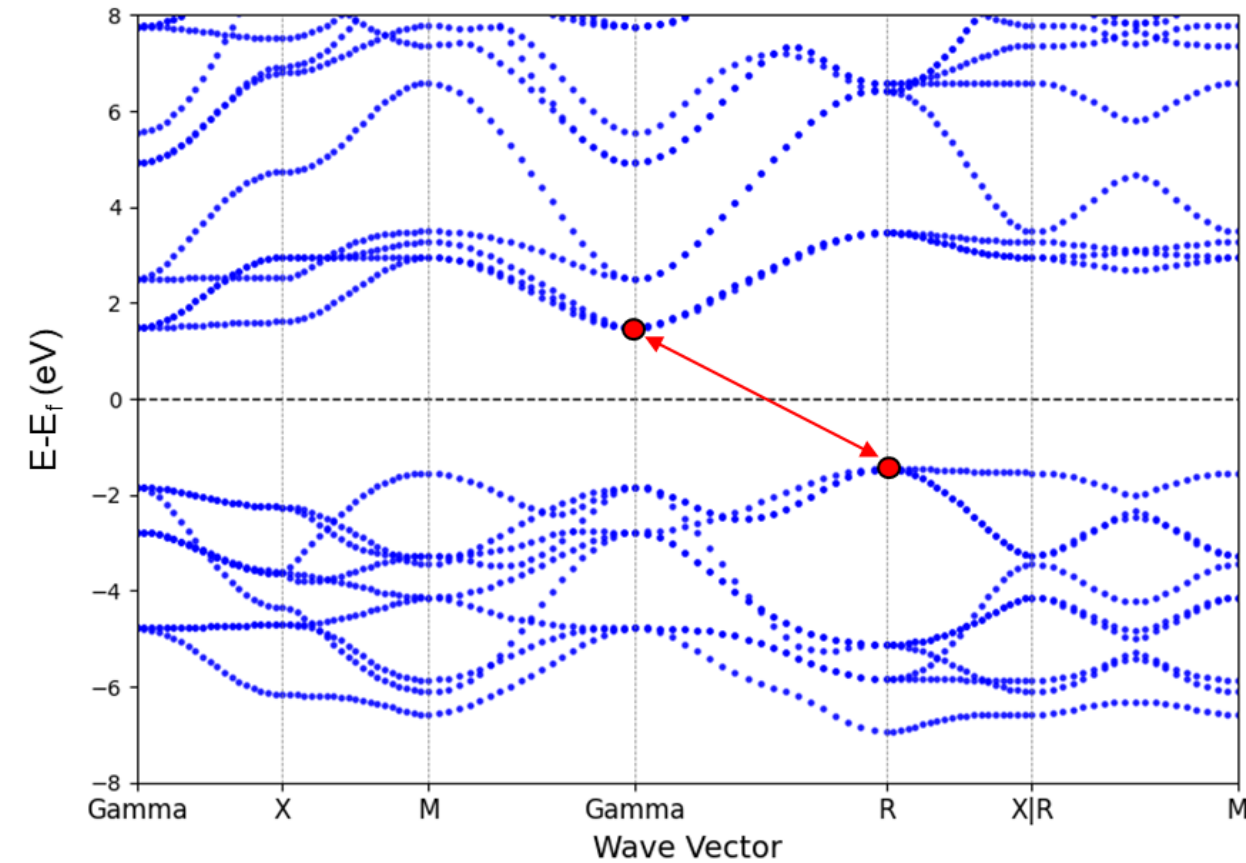
Example Case  $\text{SrTiO}_3$  (Cubic)



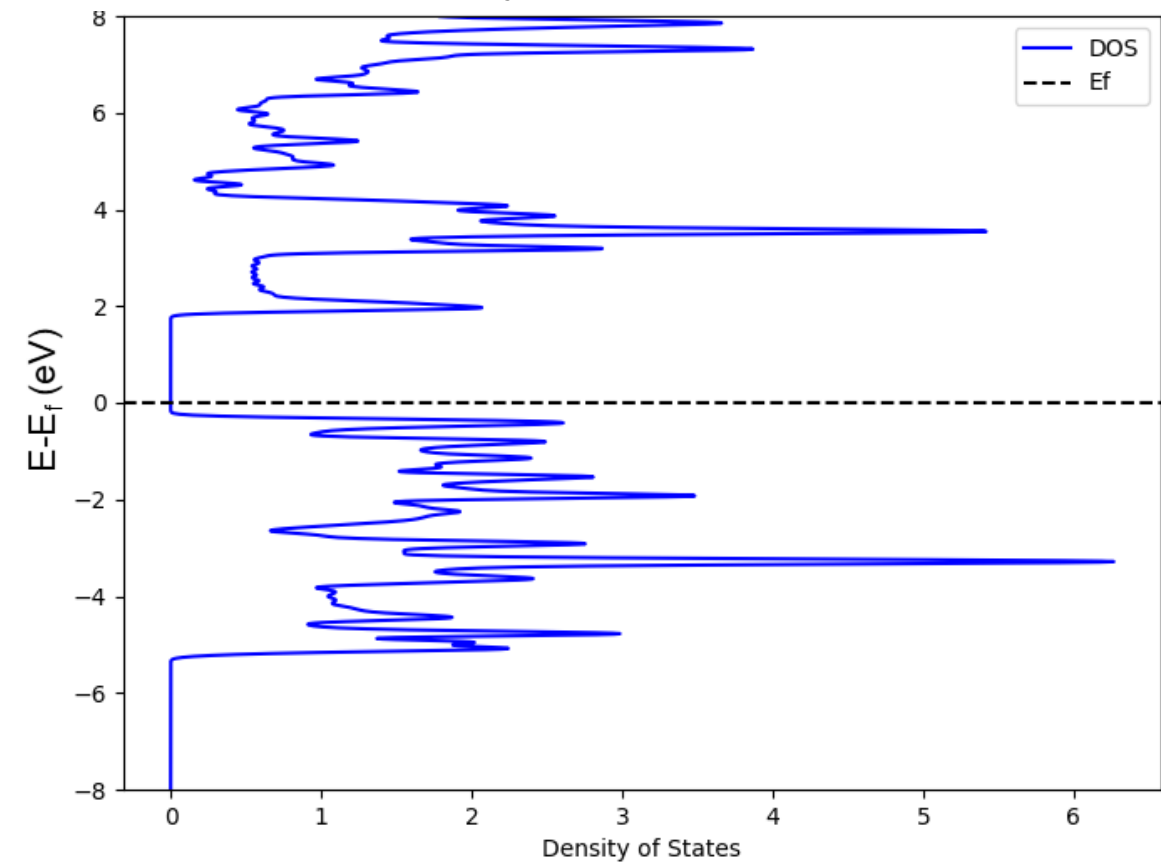
# Current Work

## Developing an AI assisted Neuromorphic Material Simulator: Example Case SrTiO<sub>3</sub> (Cubic)

### Band Structure



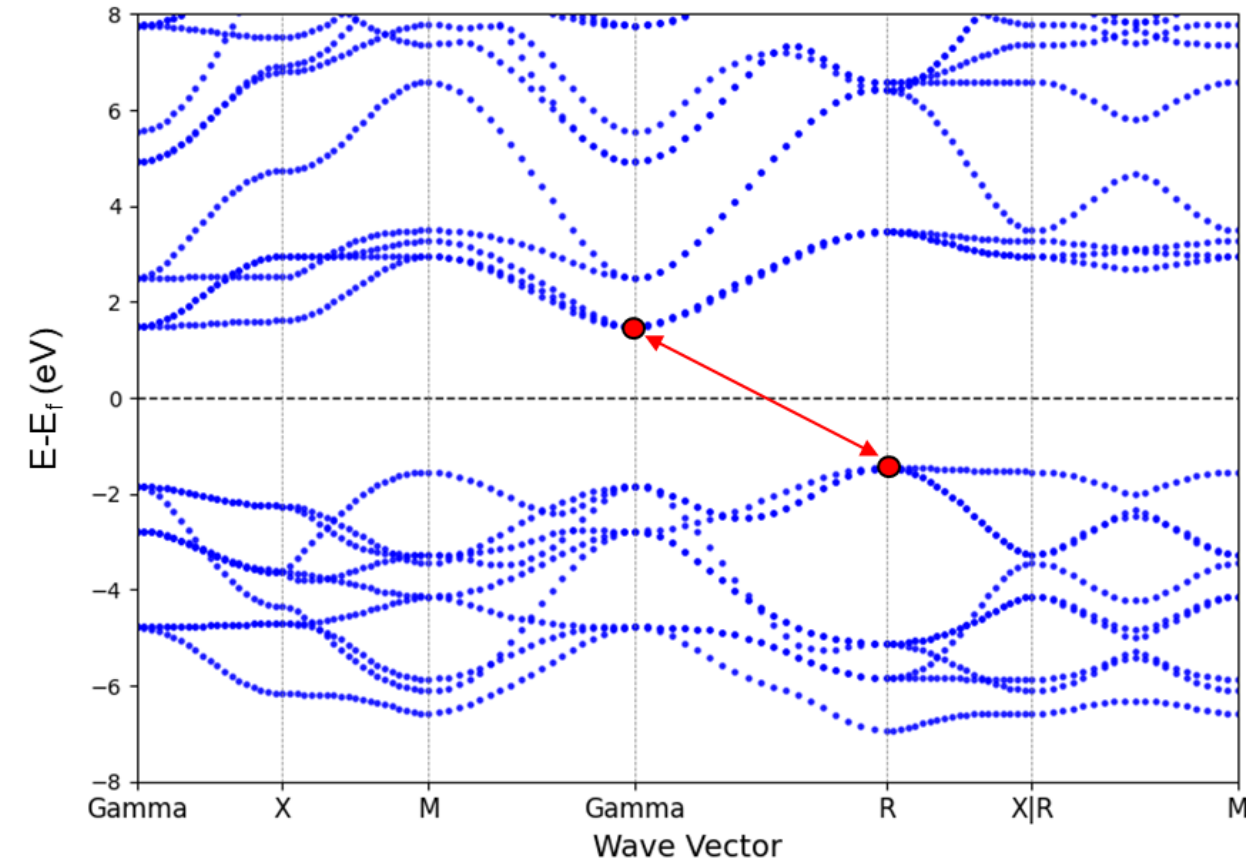
### Density of State (DOS)



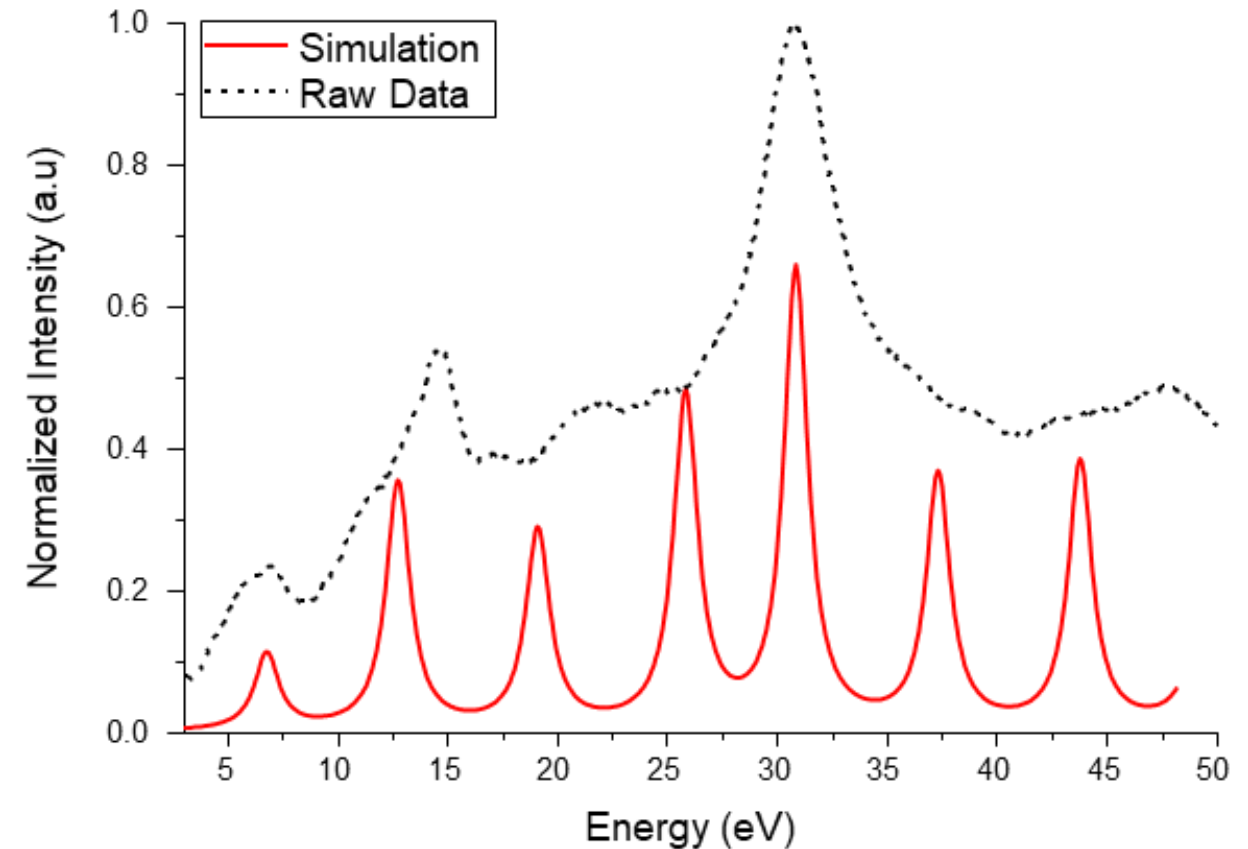
# Current Work

## Developing an AI assisted Neuromorphic Material Simulator: Example Case SrTiO<sub>3</sub> (Cubic)

### Band Structure



### EELS Low Loss Spectra







# Thank You!

[santi.barri@unizar.es](mailto:santi.barri@unizar.es)