EGI-ACE Use Case for PERLA-PV

EGI/BSUN Summer School, 2022
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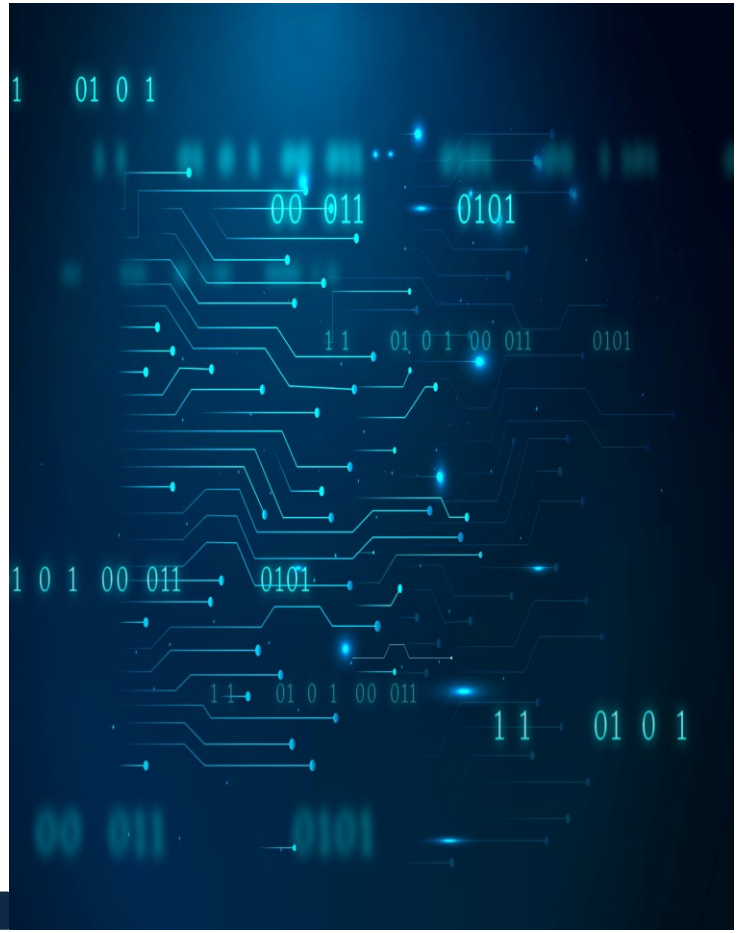
Table of Contents



Towards perovskite large area photovoltaics (PERLA-PV)

***EGI** infrastructure is used for supporting the **PERLA-PV** project.*

The project evolved from the ***European Economic Area (EEA) Grants*** and aims to develop efficient, stable, reproducible standard and inverted perovskite solar cells and photovoltaic modules fabricated with affordable large area and environmental friendly technologies, reducing to minimum the pollutants during fabrication process.

It is expected that by developing low cost and stable photovoltaic panels with optimized efficiency the use of such devices in public and private buildings such as offices, supermarkets, houses, schools, etc.

PARTNERS

Why EGI-ACE?

Advanced Computing for EOSC

EGI-ACE is a 30-month (2021-2023) project coordinated by the EGI Foundation with a mission to empower researchers from all disciplines to collaborate in data- and compute-intensive research through free-at-point-of-use services.

"***EGI-ACE's*** main objective is to implement the ***Compute Platform of the European Open Science Cloud*** and contribute to the EOSC Data Commons by delivering integrated computing, platforms, data spaces and tools as an integrated solution that is aligned with major European cloud federation projects and HPC initiatives."

https://www.egi.eu/project/egi-ace/

Applying for EGI computing services

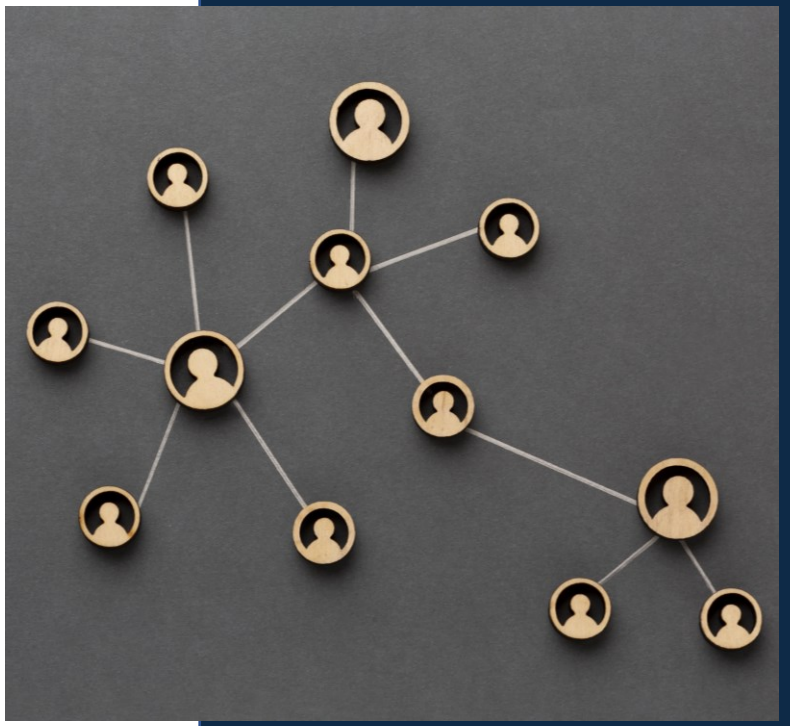
Made within the Use Cases Call

- Contacts
- Virtual Organisation/EGI Check-in
- Summary of use cases
- Resources / technical requirements
- Virtual Machine/Cluster Creation

Contacts

- ***Provider: CLOUDIFIN (IFIN-HH)***
  - Mihnea Dulea, Ionut Vasile, Dragos Ciobanu

- ***PERLA-PV Community***:
  - Department of Engineering, Reykjavik University (RU), Iceland: Andrei Manolescu, Kristinn Torfaso
  - Faculty of Physics, University of Bucharest, – Ilfov, Romania: Alexandru NEMNES, Nicolae Filipoiu



PERLA-PV Use Case Objectives

Scientific objective

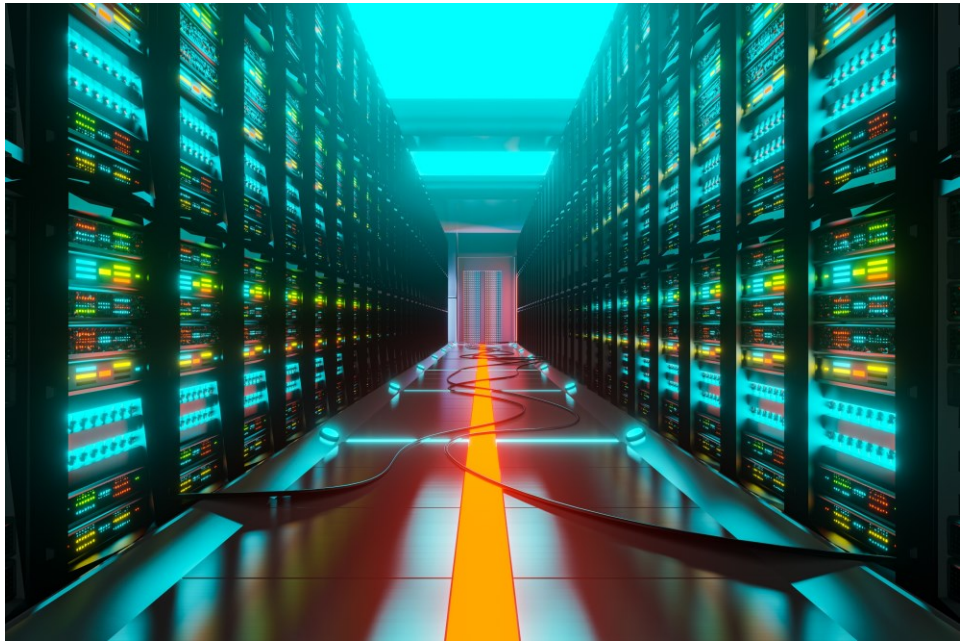
The main scientific goal is the development of combined density functional theory (DFT) and machine learning (ML) techniques to predict electronic properties of hybrid perovskite materials and interfaces, which are currently used in perovskite solar cells.

Computing objective

The computing objectives concern the implementation of the DFT calculations using specialized software packages (SIESTA code) and the implementation of artificial neural networks (ANNs) using TensorFlow library (with Keras frontend).

PERLA-PV Resources/Technical requirements

- 320 vCPUs
- Node configuration: 32 cores x 4GB RAM
- 10GB of local storage /per node
- 1 public IP
- Technical support for SLURM, MPI libraries, Tensor Flow, Keras



Summary of how we obtained acces to the EGI cloud infrastucture

01 **EGI create a new Virtual Organization for PERLA-PV project**:

- EGI contacted the provider and negotiated resources for us.
- We signed a Service Level Agreement (SLA) with EGI.
- A new Virtual Organization was created for our community.

02 **Virtual Machine/Cluster Creation for PERLA-PV**

Scientific Results using the EGI cloud infrastructure

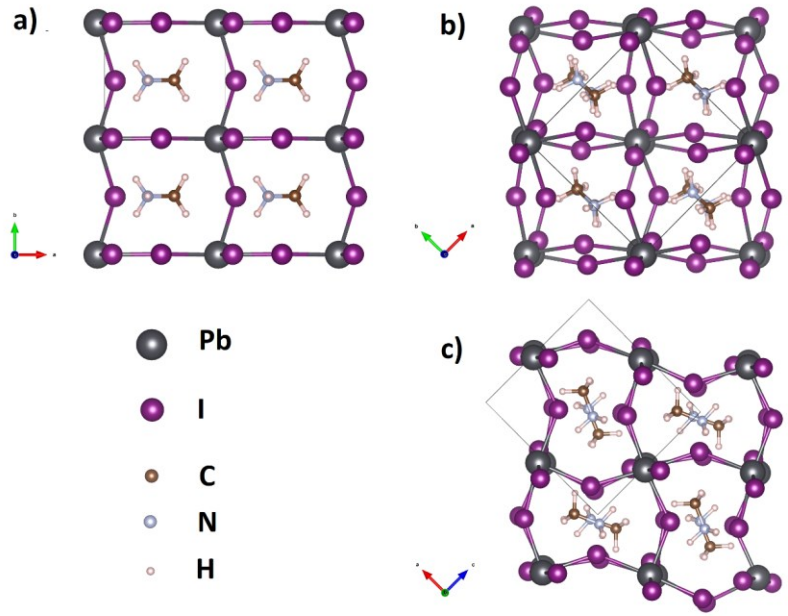
Materials Structural Optimization:

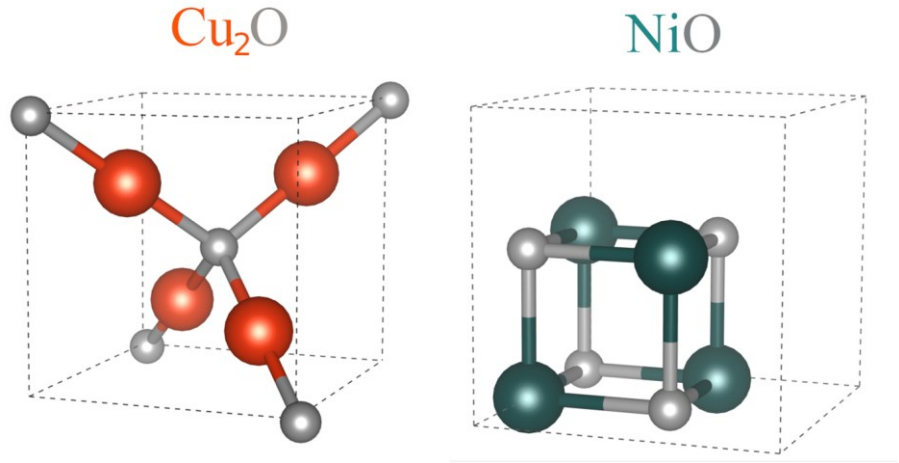
a) MAPI Cubic

b) MAPI Tetragonal

c) MAPI Orthorhombic

MAPI=CH3NH3PbI3



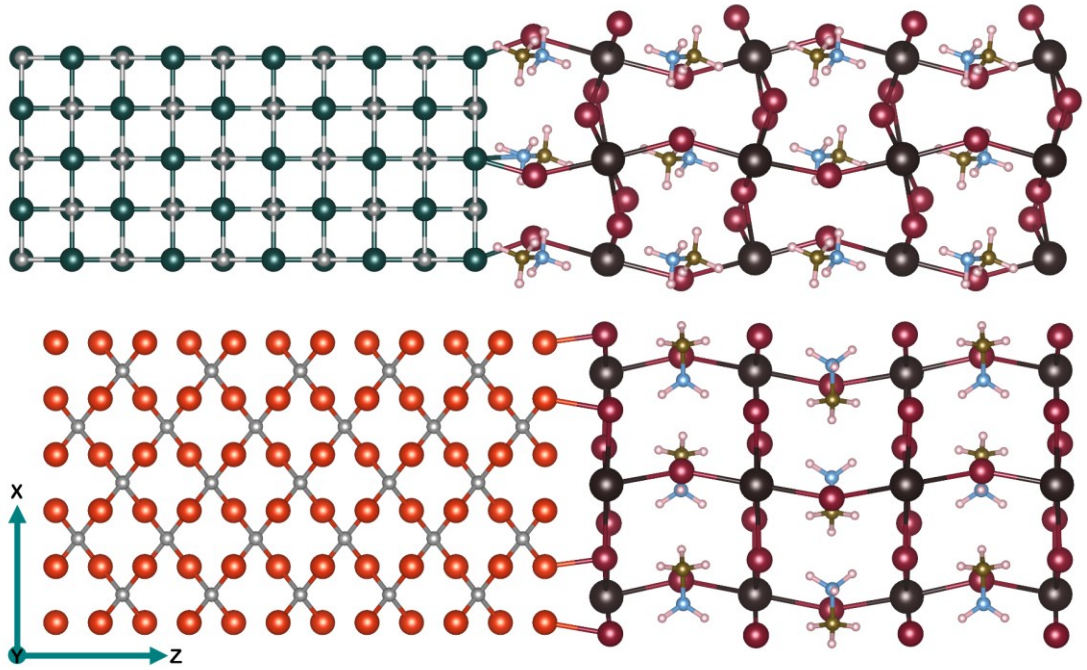


Transition-Metal Oxides

Scientific Results using the EGI cloud infrastructure

Perovskite- transition metal oxide interfaces:

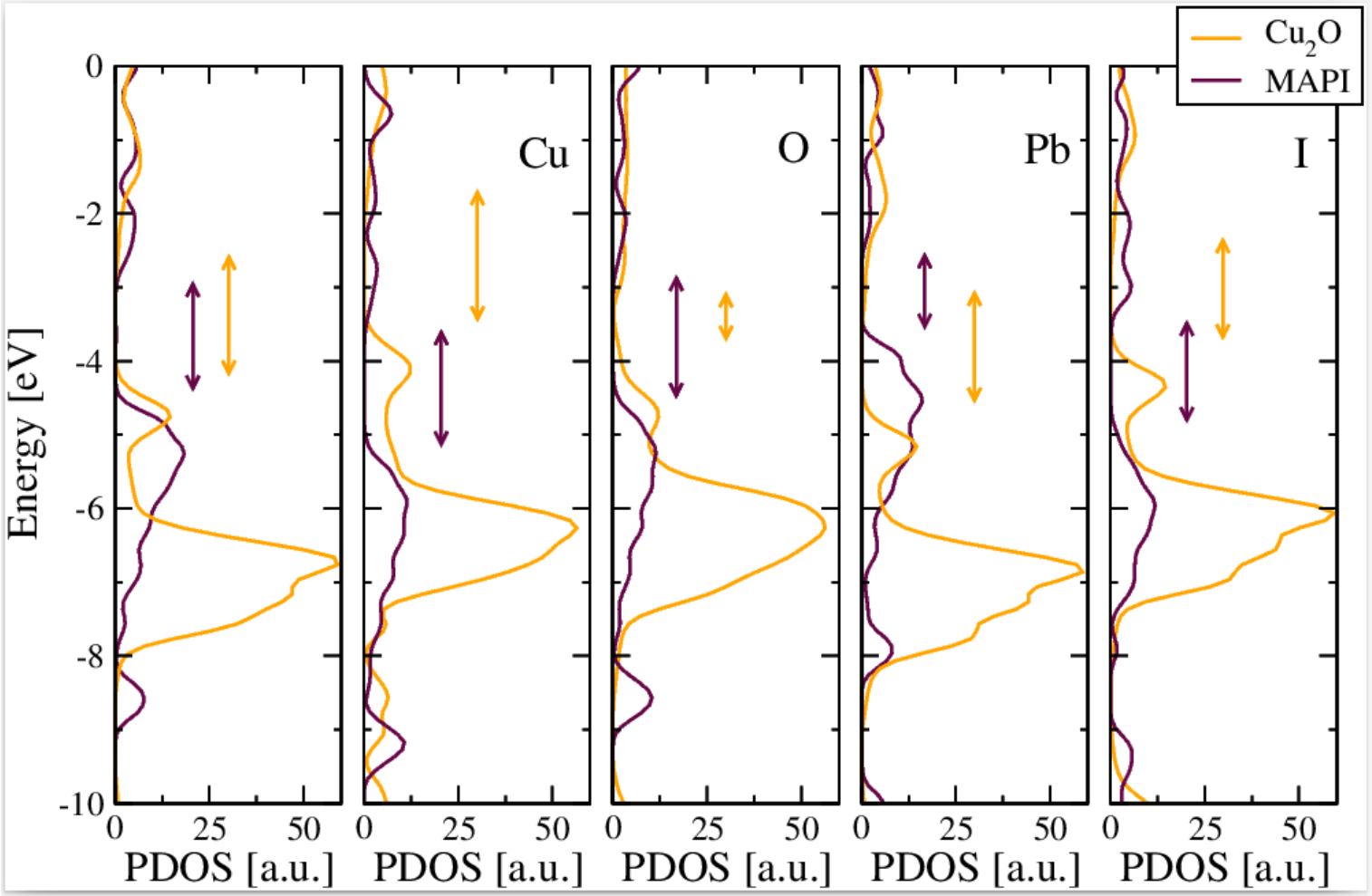
- Interface Relaxation
- Band alignment in the presence of vacancies
- Band alignment in the presence of dopants



NiO@MAPI
218 atoms

Cu2O@MAPI
256 atoms

MAPI@Cu_2O Vacancies



The band offset is:

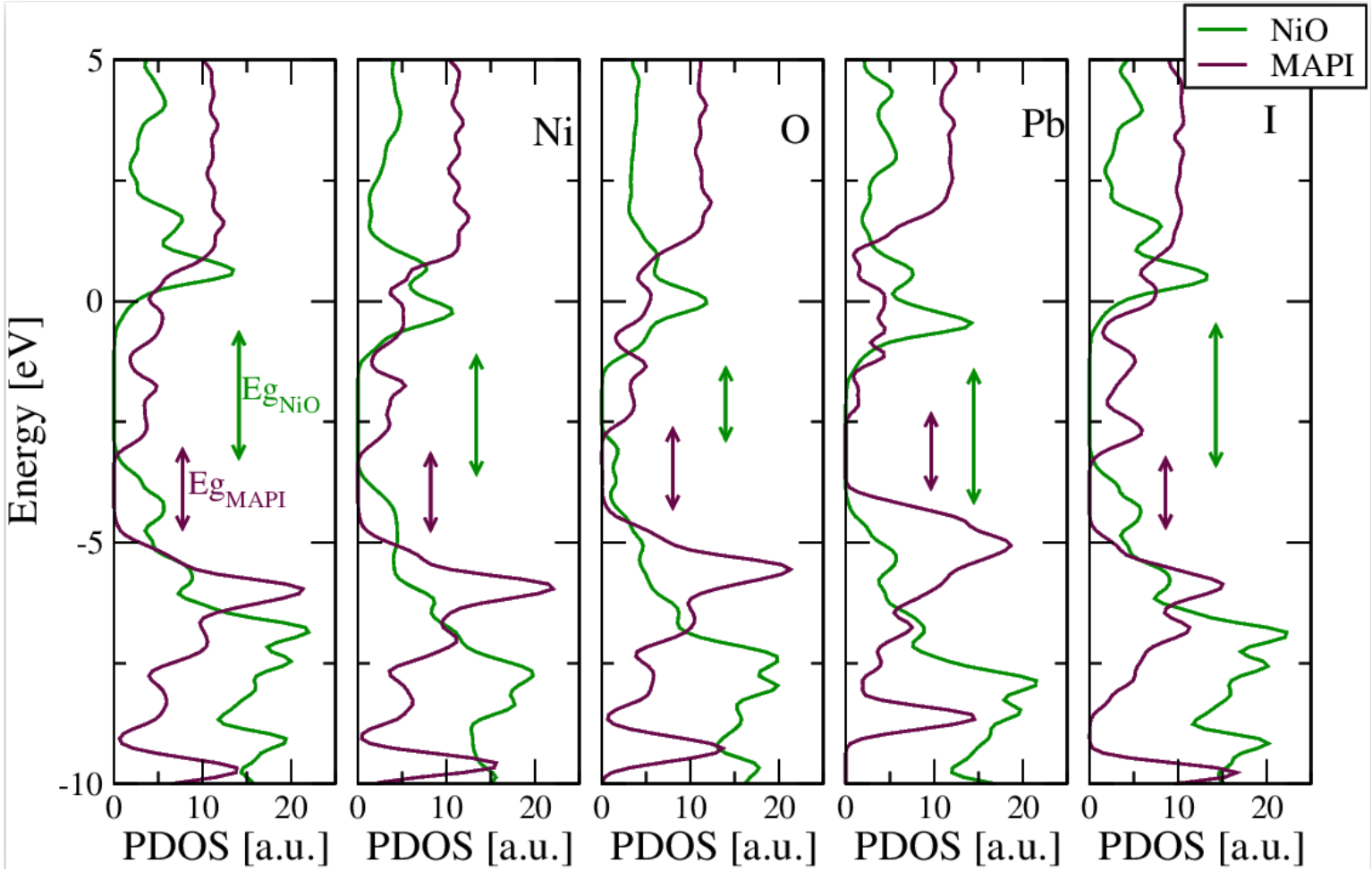
- enhanced by I and Cu
- reduced by Pb and O

MAPI@NiO Vacancies

The band offset is:

- enhanced by I vacancies
- reduced by Pb and Ni

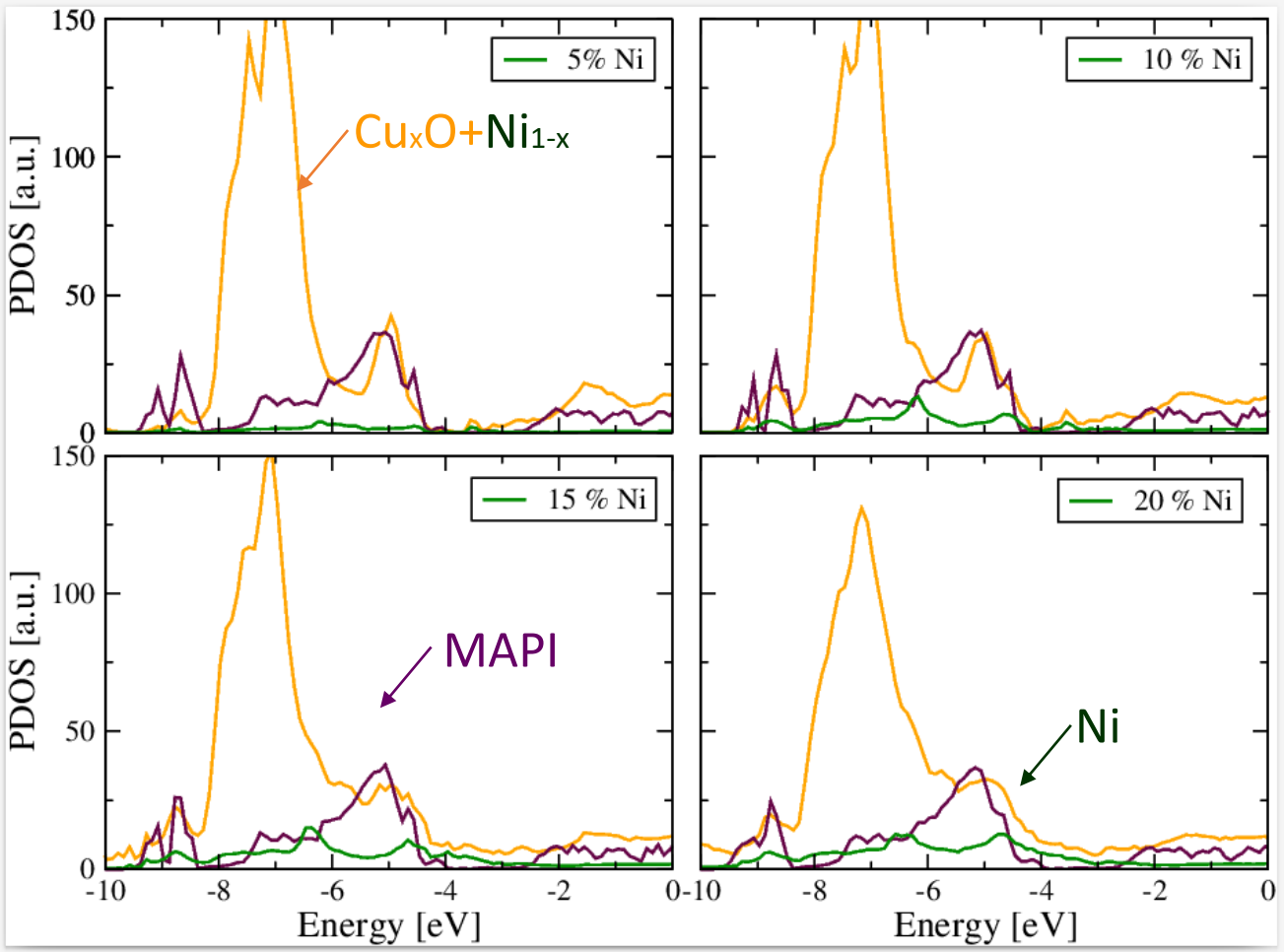
O vacancies are decreasing the NiO band gap



MAPI@$Cu_xNi_{1-x}O$

- We generated 10 random doped structures for every Ni concentration

- Ni dopants induce a p-type doping for the Cu2O band-gap



Scientific Results

- We performed structural optimizations for the bulk materials.
- Proper band structures were obtained for TMS using DFT+U.
- We analized the band alignment for the tow interfaces: MAPI@Cu2O and MAPI@NiO.
- Cu and I are beneficial for enhancing the band offset, while Pb and O vacances decrease it.
- The Ni dopants increases the hole-conducting properties of the Cu2O oxide.


THANK YOU!