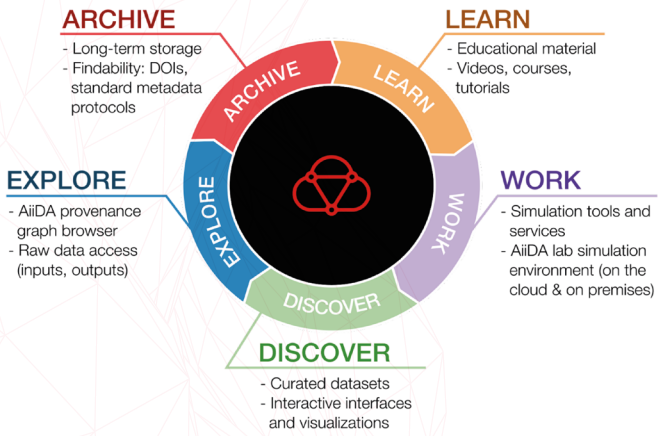
MAX DRIVING THE EXASCALE TRANSITION

MATERIALS CLOUD

Description

Materials Cloud is a platform designed to enable open and seamless sharing of resources for computational science, driven by applications in materials modelling. It is organized into five sections:

- **LEARN**, containing educational materials;
- **WORK**, which focuses on simulation services, turnkey solutions, data analytics tools;
- **DISCOVER**, containing curated data, presented via tailored interactive visualizations;
- **EXPLORE**, which allows to browse the full provenance of selected databases; and
- **ARCHIVE**, which is an open-access, moderated research data repository.

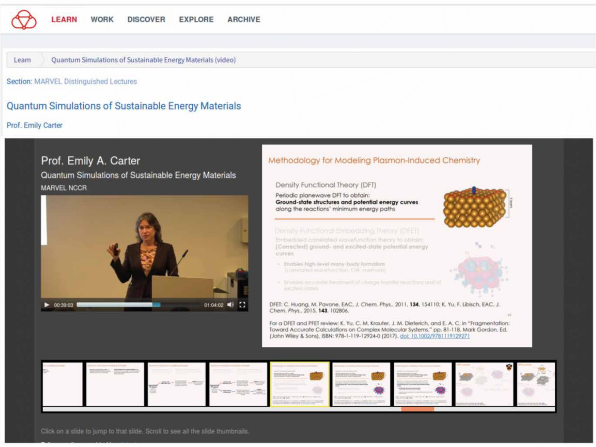


Learn

The LEARN section contains:

- > 170 talks
- > 30.000 views/year
- > 1.200 YouTube subscribers

Main sections include: MARVEL events, AiiDA & Materials Cloud tutorials, Quantum ESPRESSO & Wannier90 schools, Fireside chats.

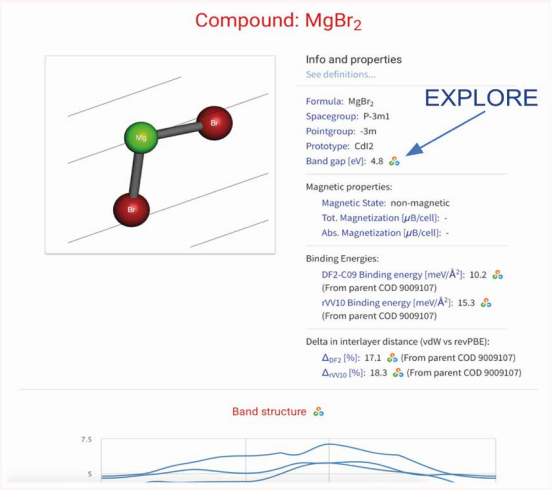


Discover & Explore

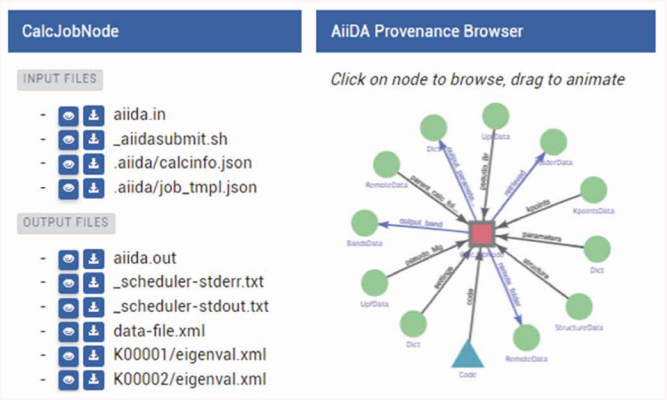
The DISCOVER section contains tailored ways of exploring curated datasets, including

- MC3D - Materials Cloud three-dimensional crystal database (Huber et al.)
- MC2D - Materials Cloud two-dimensional crystal database (Mounet, Campi et al.)
- SSSP - Standard solid-state pseudopotentials (Prandini et al.)
- 2D topological insulators (Marrazzo et al.)
- Covalent organic frameworks for methane storage applications (Mercado et al.)
- and many others.

An example DISCOVER page for a material in the MC2D database is shown below:



The various properties include links to the corresponding EXPLORE section (figure below), which contains the full provenance (all codes used, inputs and outputs, etc.) of how each specific property was calculated.



The EXPLORE browser for published databases can also be accessed directly, as well as connected to your offline AiiDA databases.

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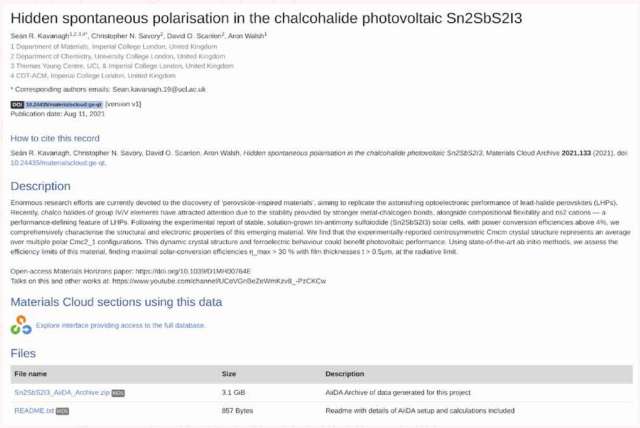
Archive

Materials Cloud Archive is an open repository for computational materials science research data. It is moderated (but not peer-reviewed) to ensure that submitted content upholds the platform-specific guidelines.

The motivation behind the archive is to help reproducing results discussed in scientific publications.
Submissions receive a persistent DOI and a guaranteed lifetime of at least 10 years.
Features include full-text search, editing of entries, and integration with external services (e.g., RenkuLab to inspect AiiDA databases).


Hidden spontaneous polarisation in the chalcohalide photovoltaic Sn2SbS2I3

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Seán R. Kavanagh, Christopher N. Savory, David O. Scanlon, Aron Walsh, *Hidden spontaneous polarisation in the chalcohalide photovoltaic Sn2SbS2I3*, Materials Cloud Archive **2021.133** (2021), doi: 10.24435/materialscloud:ge-qt.

Description

Enormous research efforts are currently devoted to the discovery of 'perovskite-inspired materials', aiming to replicate the astonishing optoelectronic performance of lead-halide perovskites (LHPs). Recently, chalco halides of group IV/V elements have attracted attention due to the stability provided by stronger metal-chalcogen bonds, alongside compositional flexibility and ns2 cations — a performance-defining feature of LHPs. Following the experimental report of stable, solution-grown tin-antimony sulfaiodide ($Sn_2SbS_2I_3$) solar cells, with power conversion efficiencies above 4%, we comprehensively characterise the structural and electronic properties of this emerging material. We find that the experimentally-reported centrosymmetric Cmcm crystal structure represents an average over multiple polar Cmc2_1 configurations. This dynamic crystal structure and ferroelectric behaviour could benefit photovoltaic performance. Using state-of-the-art ab initio methods, we assess the efficiency limits of this material, finding maximal solar-conversion efficiencies $\eta_{max} > 30$ % with film thicknesses $t > 0.5\mu m$, at the radiative limit.

Open-access Materials Horizons paper: https://doi.org/10.1039/D1MH00764E
Talks on this and other works at: https://www.youtube.com/channel/UCdVGnBeZeWmKzv8_-PzCKCw

Materials Cloud sections using this data

Explore interface providing access to the full database.

Files

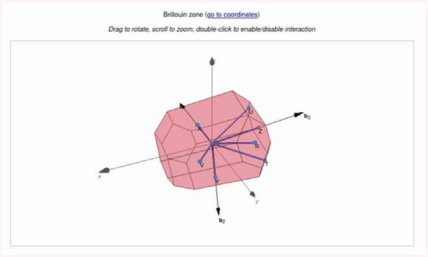
File name	Size	Description
Sn2SbS2I3_AiiDA_Archive.zip	3.1 GiB	AiiDA Archive of data generated for this project
README.txt	857 Bytes	Readme with details of AiiDA setup and calculations included

The archive currently holds more than 600 publications and is officially recommended by Open Research Europe, Nature Scientific Data, and the Swiss National Science Foundation (SNSF) for materials data.

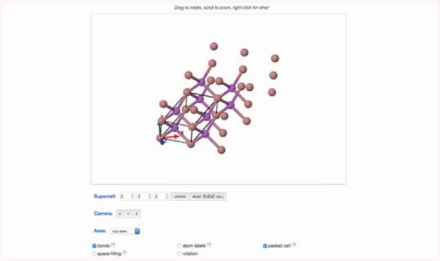
Work

The WORK section contains web-hosted tools to preprocess and analyze data or speed up research using machine learning techniques. The tools include

- Quantum ESPRESSO input generator and structure visualizer



- SeeK-path: the k-path finder and visualizer



- OPTIMADE materials database explorer
- ShiftML: chemical shifts in molecular solids by machine learning
- AlphaML: machine learning of molecular polarizabilities
- and many others.

Additionally, this section contains ***Quantum Mobile***, a virtual machine image including many common materials simulation software and the AiiDA python framework, ideal for teaching codes in schools and tutorials; and ***AiiDAlab***, a web platform that allows to run and manage complex, robust, reliable AiiDA workflows via tailored lightweight web applications.

Contact & Support

Main Website

Archive

Data management plan template

Contacts

References

- *L. Talirz, S. Kumbhar, E. Passaro et al. "Materials Cloud, a platform for open computational science." Scientific Data* ***7,*** *299 (2020). https://doi.org/10.1038/s41597-020-00637-5*

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