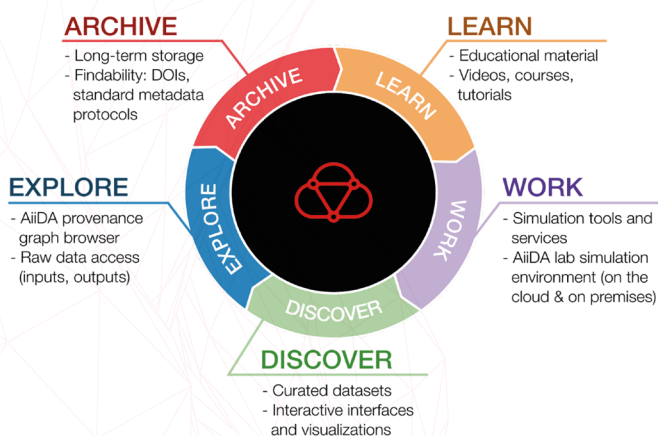


## Description

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.

Learn: Quantum Simulations of Sustainable Energy Materials (video)

Section: MARVEL Distinguished Lectures

Quantum Simulations of Sustainable Energy Materials

Prof. Emily Carter

Methodology for Modeling Plasmon-Induced Chemistry

Density Functional Theory (DFT)

Periodic plane-wave DFT to obtain ground state structures and potential energy curves along the reaction's intrinsic energy paths

Periodically extended time-dependent DFT (PE-TDDFT) to describe the excited state potential energy curves

Time-dependent many-body perturbation theory (GW) to describe the excited state potential energy curves

DFT: C. Huang, M. Pascale, EAC, J. Chem. Phys. 2011, 134, 134103; K. Fu, F. Schuch, EAC, J. Chem. Phys. 2013, 138, 103304

For a DFT and PE-TDDFT review, K. Fu, C. M. Rostler, J. M. Dabkowiak, and E. A. Carter, "Progress in Energy Materials: Calculations on Complex Molecular Systems", vol. 8, p. 18, World Scientific, (John Wiley & Sons), ISBN 978-1-119-12924-9 (2017), doi: 10.1002/9781119129249.ch08

## 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:

Compound: MgBr<sub>2</sub>

Info and properties

See definitions...

**EXPLORE**

Formula: MgBr<sub>2</sub>

Spacegroup: P-3m1

Pointgroup: -3m

Prototype: CdI<sub>2</sub>

Band gap (eV): 4.8

Magnetic properties:

Magnetic State: non-magnetic

Tot. Magnetization [ $\mu_B$ /cell]: -

Abs. Magnetization [ $\mu_B$ /cell]: -

Binding Energies:

DF2-C09 Binding energy (meV/Å<sup>3</sup>): 10.2

(From parent COD 9009107)

rVV10 Binding energy (meV/Å<sup>3</sup>): 15.3

(From parent COD 9009107)

Delta in interlayer distance (vdW vs revPBE):

$\Delta_{vdW}$  [%]: 17.1

(From parent COD 9009107)

$\Delta_{vdW}$  [%]: 18.3

(From parent COD 9009107)

Band structure

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.

CalcJobNode

AiiDA Provenance Browser

Click on node to browse, drag to animate

INPUT FILES

- aiiida.in
- \_aiidasubmit.sh
- \_aiida/calcinfo.json
- \_aiida/job\_tmpl.json

OUTPUT FILES

- aiiida.out
- \_scheduler-stderr.txt
- \_scheduler-stdout.txt
- data-file.xml
- K00001/eigenval.xml
- K00002/eigenval.xml

Provenance graph showing nodes for CalcJobNode, RemoteData, and Code.

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

## 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 chalcogenide photovoltaic Sn<sub>2</sub>Sb<sub>2</sub>S<sub>13</sub>

Seán R. Kavanagh<sup>1,2,3,4\*</sup>, Christopher N. Savory<sup>2</sup>, David G. Scantlon<sup>2</sup>, Aron Walsh<sup>1</sup>  
<sup>1</sup> Department of Materials, Imperial College London, United Kingdom  
<sup>2</sup> Department of Chemistry, University College London, United Kingdom  
<sup>3</sup> Thomas Young Centre, UCL, 8 Imperial College London, United Kingdom  
<sup>4</sup> CDT-AiDA, Imperial College London, United Kingdom

\* Corresponding authors emails: Sean.kavanagh.19@ic.ac.uk

DOI: 10.26434/chemrxiv-2021-07-01  
 Publication date: Aug 11, 2021

#### How to cite this record

Seán R. Kavanagh, Christopher N. Savory, David G. Scantlon, Aron Walsh, Hidden spontaneous polarisation in the chalcogenide photovoltaic Sn<sub>2</sub>Sb<sub>2</sub>S<sub>13</sub>, Materials Cloud Archive 2021.133 (2021), doi:10.26434/chemrxiv-2021-07-01

#### 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, chalcogenide halides of group IV/VI elements have attracted attention due to the stability provided by stronger metal-chalcogen bonds, alongside compositional flexibility and n2+ cations — a performance-defining feature of LHPs. Following the experimental report of stable, solution-grown In-antimony sulfide (Sn<sub>2</sub>Sb<sub>2</sub>S<sub>13</sub>) 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, C<sub>2v</sub> crystal structure represents an average over multiple polar C<sub>2v</sub> 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  $t > 0.5\mu\text{m}$ , at the radiative limit.

Open access Materials Research paper: <https://doi.org/10.1039/D1MT00114E>

Take on this and other works at <https://www.youtube.com/watch?v=1UCVGRkZwWk&list=PL72CKKw>

#### Materials Cloud sections using this data

Explore interface providing access to the full database.

#### Files

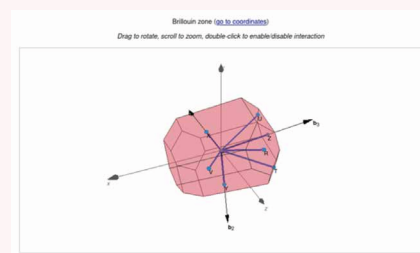
| File name                  | Size      | Description   |
|----------------------------|-----------|---|
| Sn2Sb2S13_AiDA_Archive.zip | 3.1 GiB   | AiDA Archive of data generated for this project.            |
| README.txt                 | 857 Bytes | Readme with details of AiDA setup and calculations 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.

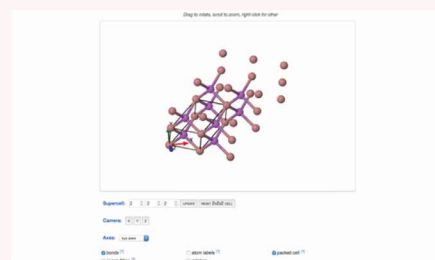
## Work

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>