



Award #: 1729297,
1728921, 1729383

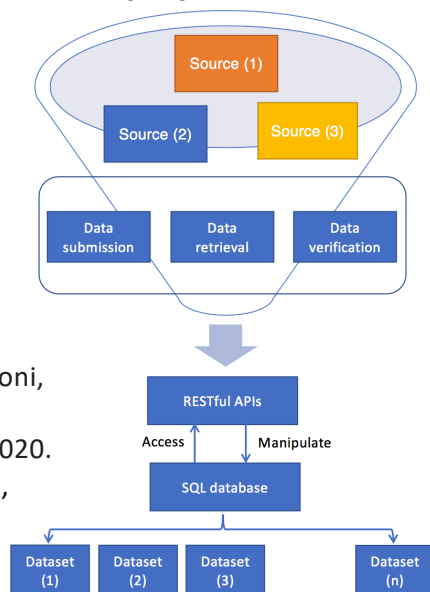
DMREF: Collaborative Research: HybriD³: Discovery, Design, Dissemination of Organic-Inorganic Hybrid Semiconductor Materials for Optoelectronic Applications

PIs: Volker Blum¹, Kenan Gundogdu², Yosuke Kanai³, David B. Mitzi¹, Franky So², Wei You³
Institutions: ¹Duke University, ²North Carolina State University, ³University of North Carolina

This project, called "HybriD³", aims to accelerate the "Design, Discovery, and Dissemination" (D³) of new crystalline organic-inorganic hybrid semiconductors. This poster will focus on the **software and data related aspects of the project**.

The underlying software, MatD³, is available for use in other, independent databases and has been integrated with the "Qresp" application ("Curation and Exploration of Reproducible Scientific Papers")

MatD³: Laasner, Du, Tanikanti, Clayton, Govoni, Galli, Ropo, Blum.
Journal of Open Source Software, 5:1945, 2020.
Qresp: Govoni, Munakami, Tanikanti, Skone, Runesha, Giberti, de Pablo, Galli.
Scientific Data, 6:190002, 2019.



Origin: computational

Lattice parameters

Crystal system: orthorhombic

a: 29.76972568 Å
b: 12.14724006 Å
c: 11.93992253 Å
α: 89.98624192°
β: 90.88085285°
γ: 89.62612599°

M. K. Jana, S. M. Janke, D. J. Dirkes, S. Dovletgeldi, C. Liu, X. Qin, K. Gundogdu, W. You, V. Blum, and D. B. Mitzi, *A Direct-Bandgap 2D Silver-Bismuth Iodide Double Perovskite: The Structure-Directing Influence of an Oligothiophene Spacer Cation*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 141, 7955-7964 (2019). doi: 10.1021/jacs.9b02909.

System description

Dimensionality: 2D
Sample type: single crystal

Computational details (click to expand)

Reference (click to expand)

Meta (click to expand)

Download data

Mint DOI

Verify data

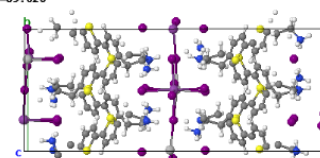
See all entries for this property (3 total)

Data set ID: 282

Report an issue

Atomic coordinates

P 1 [P 1] #1
a=29.770Å
b=12.147Å
c=11.940Å
α=89.986°
β=90.881°
γ=89.626°



JSmol

Atomic coordinates (click to expand)

NSF CSSI PI Meeting, Seattle, WA, Feb. 13-14, 2020