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

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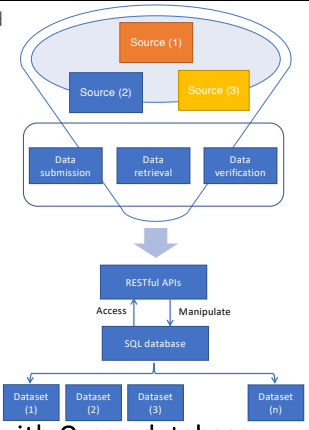
## Introduction

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.** We describe a web facing data base infrastructure "MatD3" (https://github.com/HybriD3-database/MatD3 and https://joss.theoj.org/papers/10.21105/joss.01945), a database and online presentation package for research data supporting materials discovery, design, and dissemination, developed as a generic package allowing individual research groups or projects to share materials data of any kind in a reproducible, easily accessible way. The package can be connected to the "Qresp" ("Curation and Exploration of Reproducible Scientific Papers") software (http://www.qresp.org/), which facilitates the organization, annotation and exploration of data presented in scientific papers. We finally describe the use of this infrastructure and our broader scientific activities as reflected in the open, hybrid organic-inorganic materials database "HybriD3" (https://materials.hybrid3.duke.edu/).

## MatD3 MatD³ Infrastructure

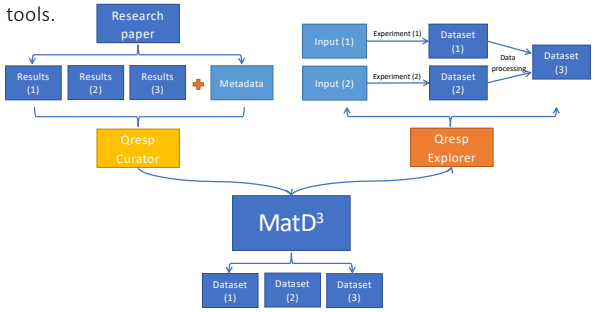
A MatD³ database is designed to **store, curate and disseminate** both experimental and theoretical materials data.

- **Database structure**: The web interface for the database is written in the Django web framework and the database itself is of the SQL type.
- **Database features:** Users can register, add data, verify submissions, and download data.




## Qresp Interaction with Qresp database

The Qresp web application (Govoni et al., 2019[13]) integrates with MatD³ to enhance the capabilities and usability of both tools.




Qresp consists of two parts:

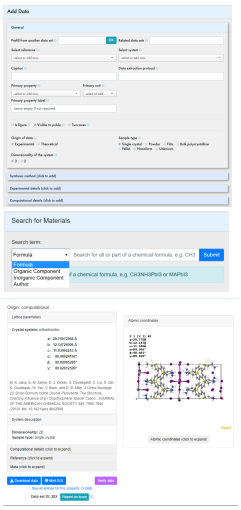
- **Curator:** guides users in the creation of metadata for the data that accompanies a publishable scientific work.
- **Explorer:** a GUI for accessing datasets, exploring workflows, and downloading curated data, published in scientific papers.

## HybriD³ HybriD³ Database

The HybriD³ database is a concrete usage of MatD³ infrastructure, predominantly for organic-inorganic hybrid perovskites.

**Database features:**

- **Add data**: Users can add experimental, computational data, synthesis method, and define and add new properties into the database
- **Curate data**: The data uploaded can be verified by other users
- **Access data**: All curated data sets are organized according to hybrid perovskite compound and can be searched by organic and inorganic compound name, formula, and authors, and can be downloaded from GUI and by RESTful API



## Functionality Demonstration

- **Curation data of the $(PEA)_2PbI_4$ structure**

- Several $(PEA)_2PI_4$ structures with different unit cell size and phase structure are reported in literatures, as shown in Table 1.

Table 1: Unit cell, structure parameters, temperature (T), space group, and disorder information of different $(PEA)_2PbI_4$ comparison.

| | Source | Unit cell | a(Å) | b(Å) | c(Å) | α | β | γ | T (K) | space group | disorder |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | C(2×2) | 8.74 | 8.74 | 33.0 | 84.7 | 84.7 | 89.6 | RT | P1̄ | Yes |
| 2 | | (1×1) | 32.51 | 6.13 | 6.19 | 90.0 | 93.8 | 90.0 | 293 | C2/m | Yes |
| 3 | | (2×2) | 12.34 | 12.22 | 32.24 | 90.0 | 94.3 | 90.0 | 100 | C1c1 | No |
| 4 | | C(2×2) | 8.68 | 8.68 | 16.41 | 94.5 | 100.6 | 90.6 | | P1̄ | Yes |
| 5 | | C(2×2) | 8.69 | 8.69 | 32.39 | 85.2 | 85.3 | 89.4 | 100 | P1̄(2) | No |
| 6 | | C(2×2) | 8.74 | 8.74 | 33.03 | 84.6 | 84.6 | 89.6 | 300 | P1̄(2) | No |
| Our work | | C(2×2) | 8.74 | 8.75 | 33.03 | 84.6 | 84.6 | 89.6 | 300 | P1̄(2) | No |

- The most stable $(PEA)_2PI_4$ structure is identified with lowest energy after structure relaxation and uploaded as curated PEPI structure data

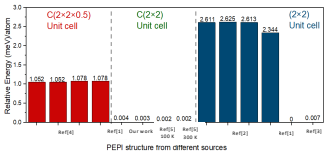



Figure 1. Relative total energy comparison between different structures with the total energy of structure from Ke-Zhao et al [1] as the reference point.

- **Comprehensive data of 2D oligoacene compounds**

Comprehensive and trustworthy data help researchers map across compounds from the same family or compare the relative progress in different perovskite families to identify any knowledge gaps in particular compounds, or any unique challenges researchers face in studying such compounds.

Table 2: Collection of oligoacene compounds $[AMA,PEA,PMA,NEA,NMA,TMA]_2PbX_4$ for X = Cl, Br or I. Compounds available on the database are shown with their data set ID and respective reference.

| | AP | BS | Abs | PL |
|---|---|---|---|---|
| **X=Cl** | | | | |
| AMA* | Exp: ID 216[6] | Comp: ID 334[7] | - | - |
| PEA* | Exp: ID 216[6] | - | Exp: PI[1] | Exp: ID 11/377[1] |
| PMA* | Exp: ID 229[8] | Comp: ID 338[7] | Exp: PI[1] | Exp: ID 8/385[1] |
| NEA[#] | - | - | - | - |
| NMA* | Exp: ID 230[8] | Comp: ID 339[7] | Exp: PI[1] | Exp: ID 13/386[1] |
| TMA[#] | - | - | - | - |
| **X=Br** | | | | |
| | AP | BS | Abs | PL |
| AMA | Comp: ID 242[7] | Comp: ID 346[7] | - | - |
| PEA | Exp: ID 227[11] | - | Exp: PI[1] | Exp: ID 10/381[1] |
| PMA | Exp: ID 224[1] | Comp: ID 336[7] | Exp: PI[1] | Exp: ID 7/380[1] |
| NEA | Exp: ID 226[1] | - | Exp: PI[1] | Exp: ID 15/382[1] |
| NMA | Exp: ID 223[1] | Comp: ID 335[7] | Exp: PI[1] | Exp: ID 12/379[1] |
| TMA | Comp: ID 245[7] | Comp: ID 349[7] | - | - |
| **X=I** | | | | |
| | AP | BS | Abs | PL |
| AMA | Comp: ID 243[7] | Comp: ID 347[7] | - | - |
| PEA | Exp: ID 225[1] | - | Exp: PI[1] | Exp: ID 9/381[1] |
| PMA | Exp: ID 228[12] | Comp: ID 337[7] | Exp: PI[1] | Exp: ID 6/384[1] |
| NEA | Exp: ID 222[1] | - | Exp: PI[1] | Exp: ID 14/378[1] |
| NMA | Comp: ID 244[7] | Comp: ID 348[7] | - | - |
| TMA | Comp: ID 246[7] | Comp: ID 350[7] | - | - |

* bis(2-aminobutylmethylammonium) # phenylethylammonium ^ phenylmethylammonium ^ 1-(2-naphthyl)ethylammonium ^ 1-(2-naphthyl)methylammonium ^ TBD

- **Metadata of phase transition temperature of $MAPbI_3$**

The metadata for the orthorhombic-tetragonal (O-T) phase transition across powder, crystal, and thin-film samples using a myriad of measurement techniques illustrates the dependence of a phase transition temperature on sample type and research interest evolution over time.

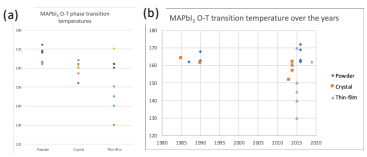



Figure 2: (a) $MAPbI_3$ orthorhombic-tetragonal phase transition temperature data compared across sample types. (b) $MAPbI_3$ orthorhombic-tetragonal phase transition temperature data taken from literature spanning from 1980s to 2010s.

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