



OPTIMADE

Open Databases Integration
for Materials Design

Presented by:

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<https://optimade.org>



16th Virtual Plenary Meeting,
11/11/2020

UCLouvain/University of Cambridge

What is OPTIMADE?

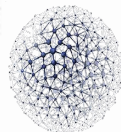


The Open Databases Integration for Materials Design (OPTIMADE) consortium aims to make materials databases interoperational by developing a common REST API.

- ❖ 4 annual meetings (est. 2016)
- ❖ 54 authors/attendees
- ❖ 19,779 words
- ❖ ~15 registered providers



**The Materials
Project**



AFLOW
Automatic - FLOW for Materials Discovery

httpk



MATERIALSCLOUD



OPTIMADE 1.0 (released July 2020)

❖ **REST API specification for common access to crystal structure databases**

- Human-readable specification (~20k words)
- Based on JSON API
- Machine-readable OpenAPI 3.0 schema

❖ **Enables unified access to 25M crystal structures from 14 providers***

- Federated providers list and discoverability mechanisms
- API validation beyond OpenAPI through associated tooling

❖ **Features:**

- Standardised representation for crystal structures, bibliographic references and links
- Well-defined grammar/filter language
- Introspective /**info** endpoint for extensibility
- API version negotiation
- Strict response format, but data models are flexible where necessary



The Specification

<https://github.com/Materials-Consortia/OPTIMADE>

optimade-python-tools

An open source Python package for consuming and implementing OPTIMADE REST APIs.



- ❖ Spin-up OPTIMADE API with “no code”
 - Built with `pydantic` and `FastAPI`
 - Annotated data models with data validation
 - Auto-generated OpenAPI 3.0 schema
 - EBNF grammar implementation with filter transformers for MongoDB & Elasticsearch
 - Mappers between existing formats and OPTIMADE, supporting aliases etc.
- ❖ Used by Materials Project and Materials Cloud
- ❖ Provides tools for validating remote implementations
- ❖ Library for client development
 - <https://dev-tools.materialscloud.org/optima-declient> Casper Andersen, EPFL



optimade-python-tools

<https://github.com/Materials-Consortia/optimade-python-tools>



OPTIMADE Providers

<https://optimade.org/providers>

<https://www.optimade.org/providers-dashboard>



What's next for OPTIMADE?

❖ OPTIMADE v1.1

- 2021 workshop - all welcome!
- Property standardization
- Trajectories
- Federated namespaces, e.g. “**_dft_**”

❖ Improved tooling:

- Continued development of **optimade-python-tools**
- Support more backends
- Enhance library functionality for creating client apps
- Closer alignment with possible use cases

❖ Semantic interoperability:

- “An Ontology for the Materials Design Domain”, Li *et al.* [arXiv:2006.07712](https://arxiv.org/abs/2006.07712)
- Fostering links with European Materials Modelling Ontology (EMMO)

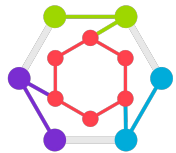
❖ Your contributions!

- CECAM OPTIMADE postdoc @ **EPFL** <https://www.cecam.org/> -> careers. Focus on molecular dynamics and biomolecular simulations
- Monthly meetings, 2021 workshop, online forum, GitHub

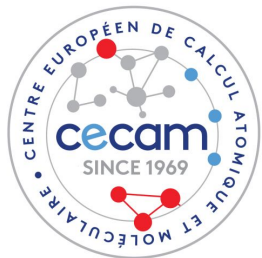
Possible avenues for discussion



- ❖ How does OPTIMADE relate to FAIR?
- ❖ How can we make the most of this federated model?
- ❖ Interoperability beyond just structure databases
- ❖ Ergonomics of research data management



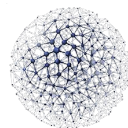
Acknowledgements



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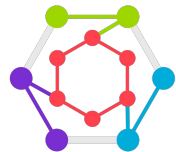
The Materials Project



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Martin Uhrin
Pierre Villars
David Waroquiers
Donald Winston
Chris Wolverton
Michael Wu
Yibin Xu
Xiaoyu Yang



Useful links

- ❖ <https://optimade.org>
- ❖ <https://optimade.org/optimade-python-tools>
- ❖ <https://github.com/Materials-Consortia>
- ❖ Forum: <https://matsci.org/c/optimade>
- ❖ Validation:
 - <https://www.optimade.org/providers-dashboard/>
 - <https://github.com/Materials-Consortia/optimade-validator-action>
- ❖ Web clients with rich interfaces:
 - <https://dev-tools.materialscloud.org/optimadeclient> Casper Andersen, *EPFL*
 - <https://optimade.science> Evgeny Blokhin, *Tilde Materials Informatics Lab*