

AFLOW: Automated infrastructure for computational materials discovery

Welcome to AFLOW, a globally available database of **2,118,033** material compounds with over **261,698,399** calculated properties, and growing.

AFLOW also offers online applications for property predictions using machine learning, crystal prototype databases, and the generation of convex hulls.

Enter an ICSD Number, AFLOW Unique Identifier, or advanced search string (e.g. Mg & Sn & Cu) to search our database.

ICSD#, AUID#, search string...

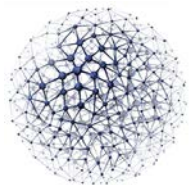
Search

Apps and Docs

AFLOW is a globally available database of **1,797,520** material compounds - with over **177,954,480** calculated properties (and growing).

CORMAC TOHER,
Corey Oses,
David Hicks,
Frisco Rose,
Eric Gossett,
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Materials Science
Duke University

Duke
UNIVERSITY



AFLOW
Automatic - FLOW for Materials Discovery



AFLOW database

The screenshot shows the AFLOW database homepage. At the top, the AFLOW logo is displayed with the tagline "Automatic - FLOW for Materials Discovery". A navigation bar includes links for HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. A welcome message states: "Welcome to AFLOW, a globally available database of **2,844,669** materials compounds with over **506,351,082** calculated properties, and growing." Below this, a grid of boxes lists various property categories and their counts: band structures (323,395), Bader charges (80,812), elastic properties (5,546), thermal properties (5,534), binary systems (1,620), binary entries (351,449), ternary systems (30,031), ternary entries (1,963,013), quaternary systems (150,620), and quaternary entries (450,554). A section titled "AFLOW also offers online applications for property predictions using machine learning, crystal prototype databases, and the generation of convex hulls." follows, with a search bar for ICSD#, AUID#, or search strings. The "Apps and Docs" section features a grid of icons for MendelLib search, Elastic properties, Thermal properties, AFLOW-ML, Crystal prototypes, AFLOW-CHULL, AFLOW-online, Binary alloy library, Superalloys search, AFLOW REST-API WIKI, AFLOW++, and PAOFLOW. The footer contains logos for Duke University, U.S. Department of Energy, Homeland Security, CRAY, and UNT.

AFLOW
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HOME | CONSORTIUM | PUBLICATIONS | FORUM | SRC | SEARCH

Welcome to AFLOW, a globally available database of **2,844,669** materials compounds with over **506,351,082** calculated properties, and growing.

323,395 band structures	80,812 Bader charges	5,546 elastic properties	5,534 thermal properties
1,620 binary systems	351,449 binary entries	30,031 ternary systems	1,963,013 ternary entries
150,620 quaternary systems		450,554 quaternary entries	

AFLOW also offers online applications for property predictions using [machine learning](#), [crystal prototype databases](#), and the generation of [convex hulls](#).

Enter an ICSD Number, [Aflowlib Unique Identifier](#), or advanced search string (e.g. Mg & Sn & Cu) to search our database.

ICSD#, AUID#, search string... **Search**

Apps and Docs

MendelLib search	Elastic properties	Thermal properties	AFLOW-ML
Crystal prototypes	AFLOW-CHULL	AFLOW-online	Binary alloy library
Superalloys search	AFLOW REST-API WIKI	AFLOW++	PAOFLOW

Duke U.S. DEPARTMENT OF ENERGY Homeland Security CRAY THE SUPERCOMPUTER COMPANY UNT

**> 500 million
properties**

**> 2.8 million
entries**

**Advanced
Search**

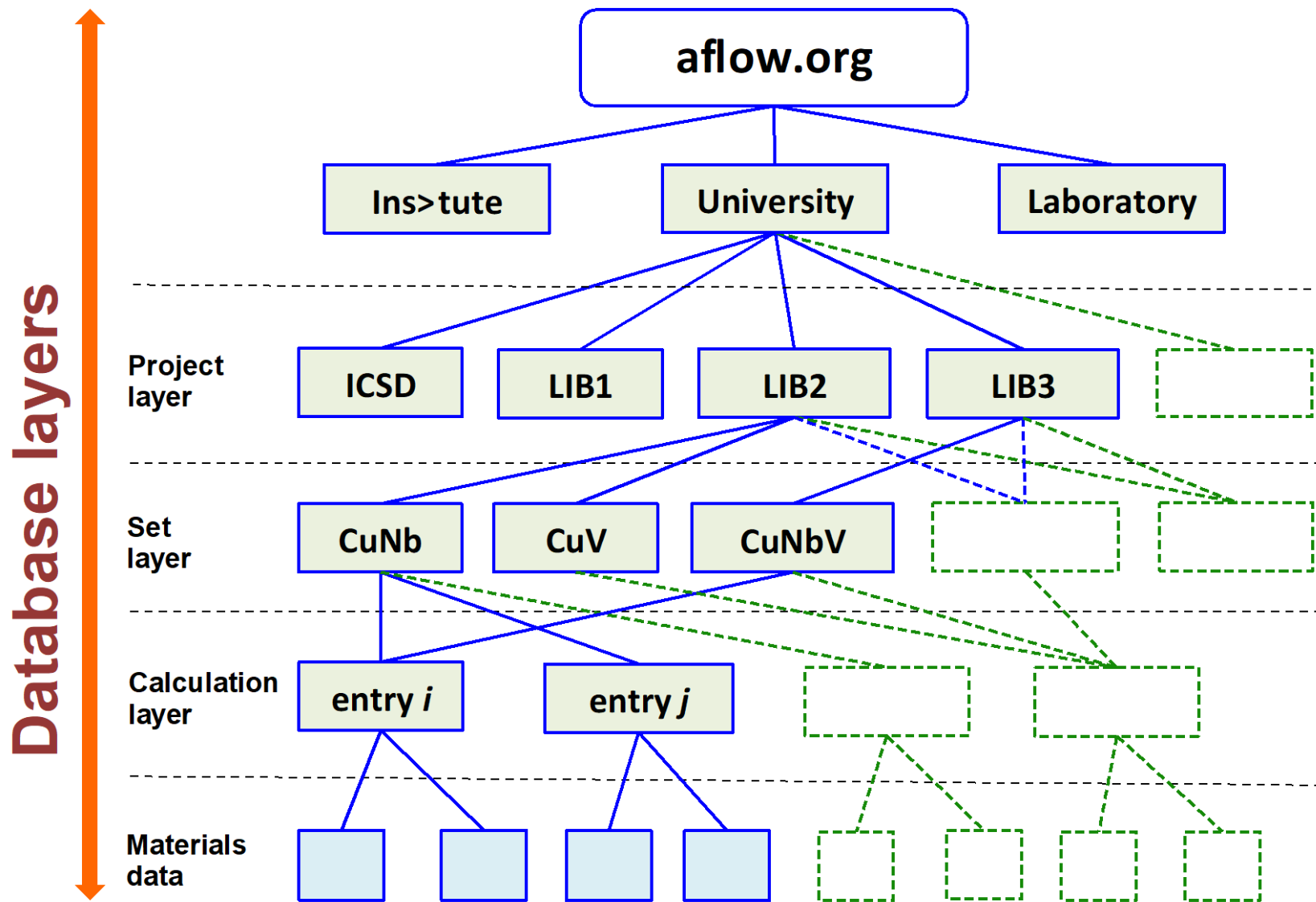
**Crystal
Prototypes
Library**

**AFLOW-ML
Online**

**Convex hull
generator**

<http://aflow.org>

AFLOW: database organization



AFLUX: AFLOW Search-API

- Enables programmatic search access through query part of URI

Logical operator	AFLUX syntax	Operator scope
<block>	"(" and ")"	Intra- and inter-property
<AND>	","	Intra- and inter-property
<OR>	":."	Intra- and inter-property
<NOT>	"!"	Intra-property
<loose>	"*"	Intra-property
<string>	""	Inter-property
<mute>	"\$"	Intra-property

[http://aflowlib.duke.edu/search/API/?species\(\(Na:K\),Cl\),nspecies\(2\),Egap\(1*,*5\)](http://aflowlib.duke.edu/search/API/?species((Na:K),Cl),nspecies(2),Egap(1*,*5))

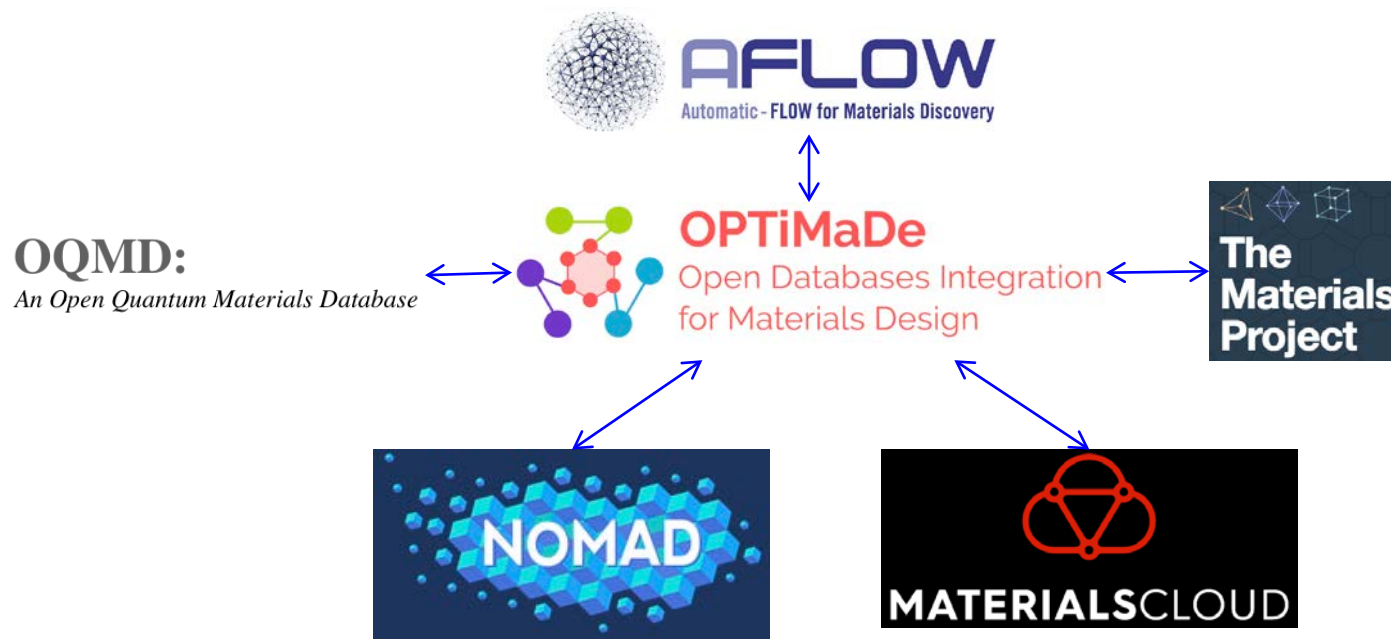
Search API Server

Query

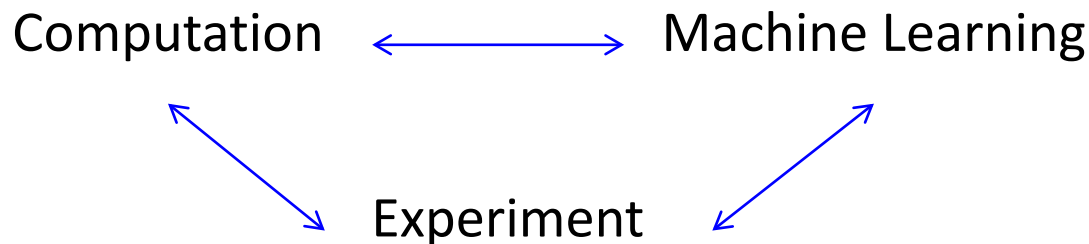
- Submit query using UNIX utility (wget, cURL); Python (urllib); etc.

Future Directions

- Common materials data API (OPTiMaDe):



- First principles computation – AI - experiment integration and feedback loops:



Acknowledgements

- Prof. Stefano Curtarolo, Director, Center for Materials Genomics
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