

COMPUTATIONAL MATERIALS REPOSITORY

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CMR Background & Application Examples

Introduction

CMR is described in:

- The Computational Materials Repository
Accepted by Comput. Sci. Eng., 2012

CMR was used in:

- Computational Screening of Perovskite Metal Oxides for Optimal Solar Light Capture
Energy Environ. Sci., vol. 5, 2012
- Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project
J. Chem. Phys., vol. 131, 2009

Introduction

State of the Art:

Calculate *electronic structure* properties of materials and analyze and handle the amount of the data by implementing a micro-solution tailored to solve that specific problem for a specific environment.

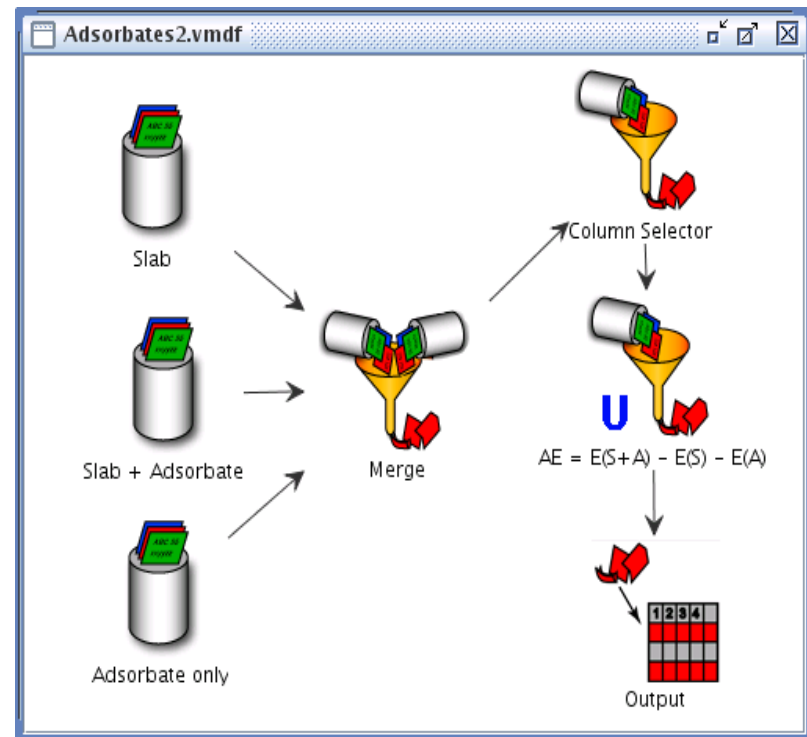
Problems:

- hard to find errors
- data exchange mostly with spread-sheets
- same problems are solved multiple times

Introduction

Solutions in 2008:

- Virtual Materials Design Framework (VMDF): Visualized queries, but did not address other issues.



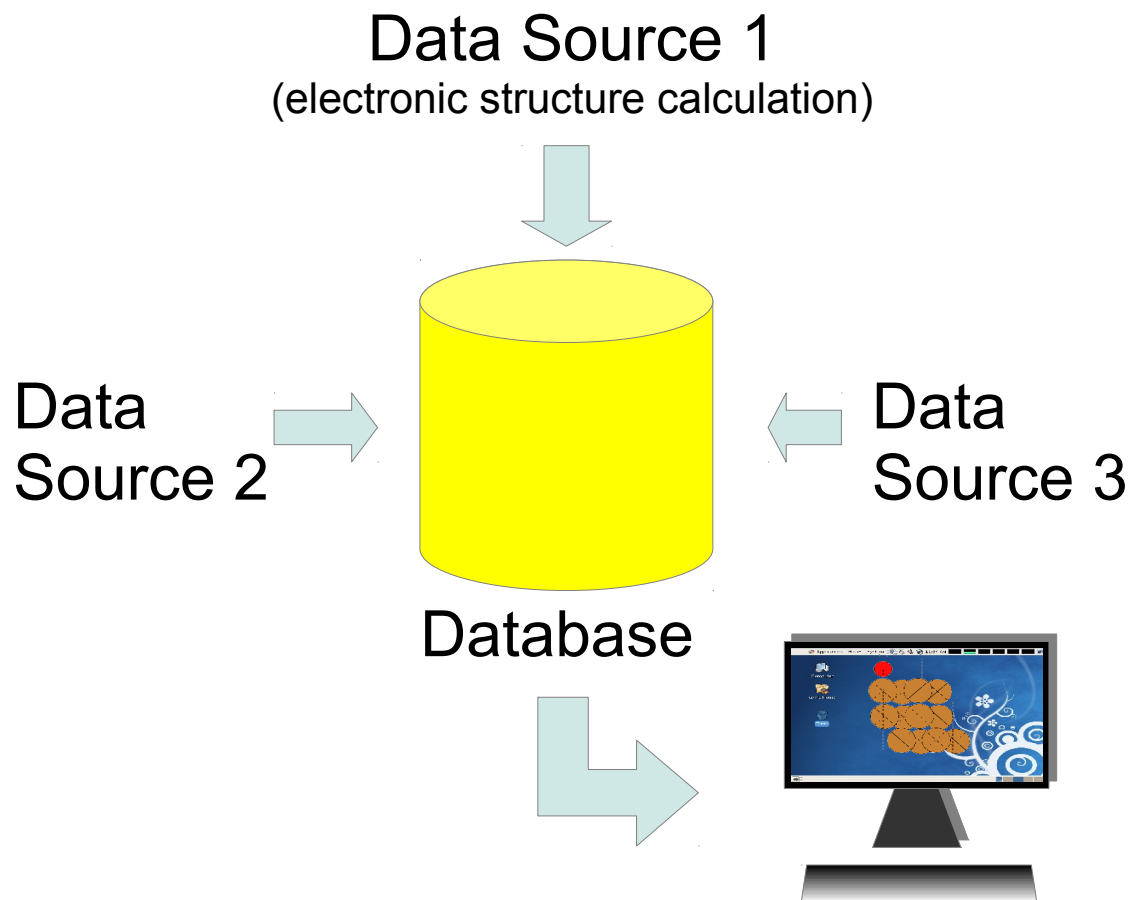
Aim of CMR

Requirements for CMR:

- Long term storage
- Structured data organization
- Re-useable methodologies
- Traceable results
- Programmable Access
- Sharing data with 3rd parties
- Presentation of results

Aim of CMR

How it's required to work:



Open Questions:

- Software
- Hardware
- Data transfer (format)
- Interfaces
- Analysis

Decisions - Software




	Python	Java	Fortran	C
LOC*	++	+	--	--
Speed	-	+	++	++
Ease of learn	++	+	-	-
Used in research	++	+	++	+
Popular (actively maintained)	++	+	?	++

*lines of code

Decisions - Software

Database software:

- relational databases 
- object databases
- no-sql databases

MySQL: safe choice: actively maintained

Decisions - Software

- Web – Server:

Apache:

actively maintained, many modules, most popular browser since 1996

→ LAMP (Linux, Apache, MySQL, PHP)

Decisions - Hardware

CMR should run on:

Laptop

- small single user project
- easy to install

Desktop

- all features
- requires database & web-server

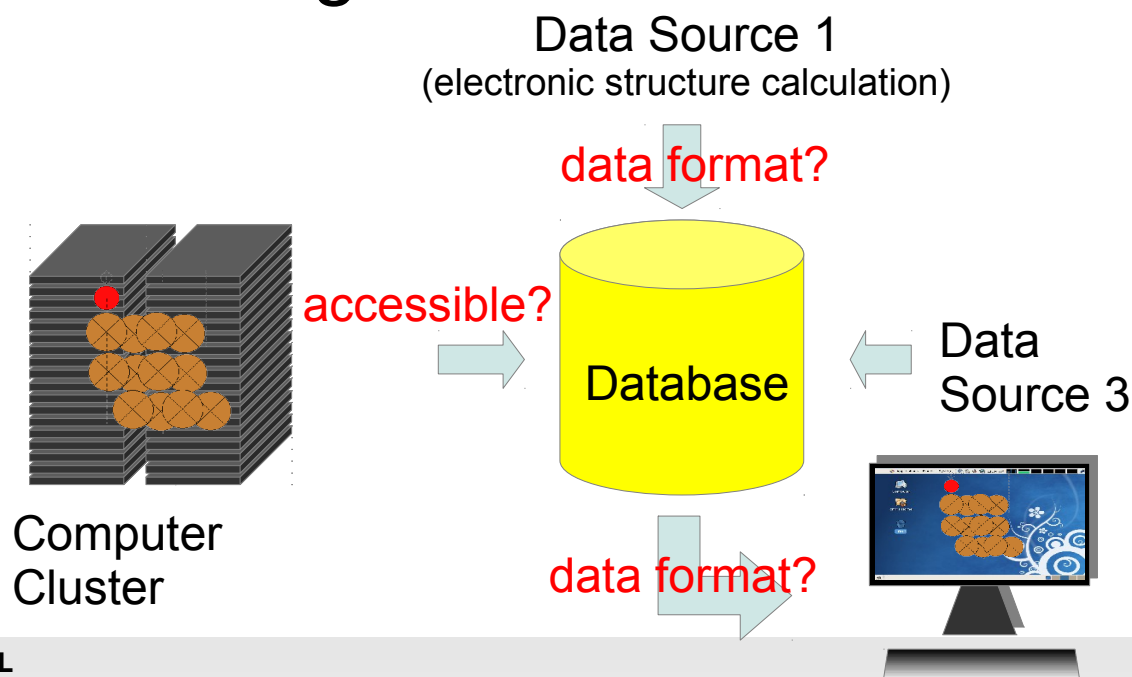
Client Server

- big database
- run on different machines

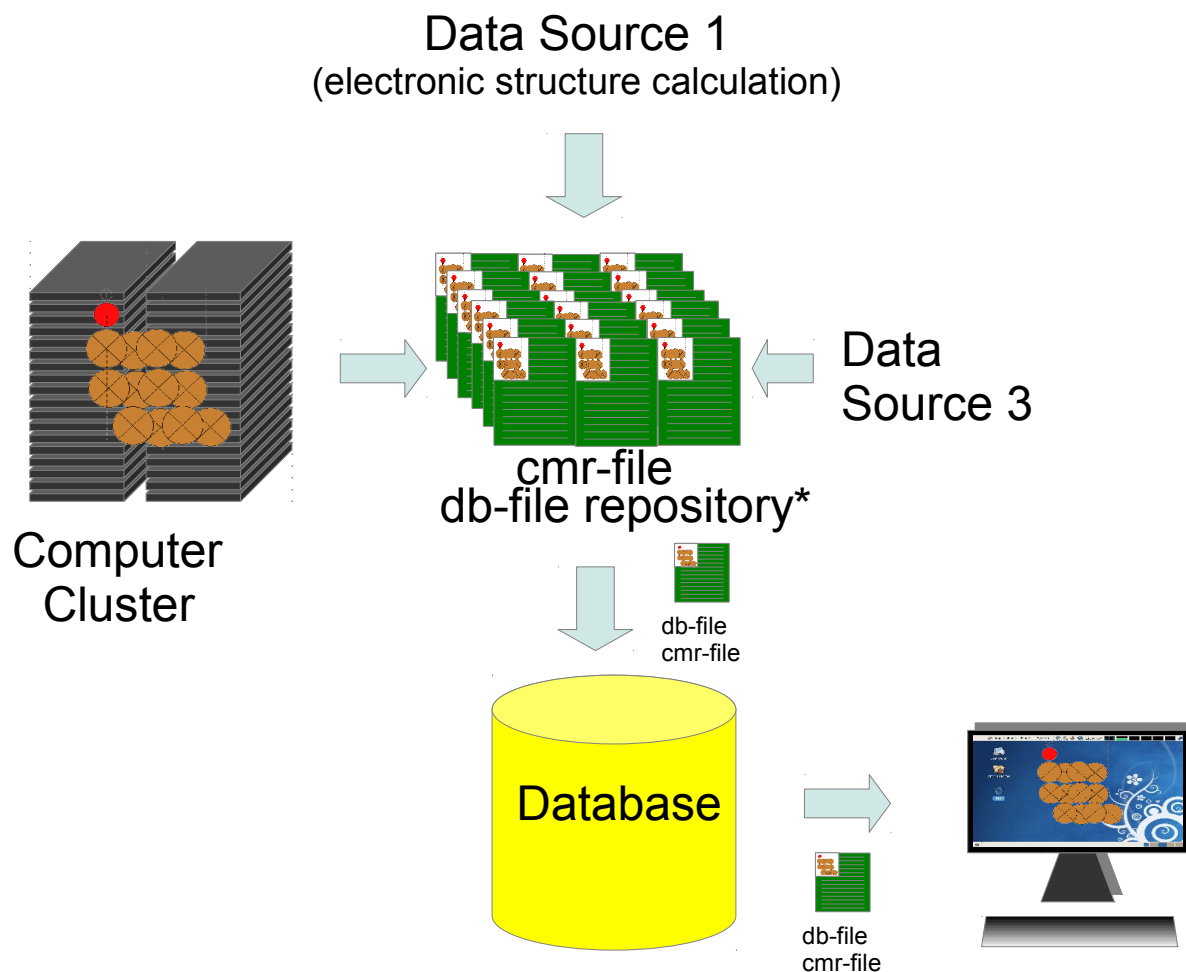
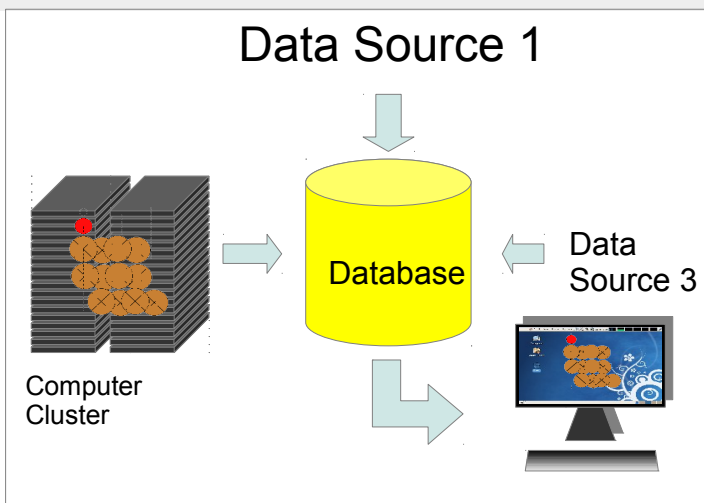
Decisions – Data Transfer

Problems:

- cannot support all foreign file formats (and all different versions of it)
- how to cope with type issues (int, numpy.int32,...)
- database might not be reachable from everywhere



Decisions – Data Transfer



Decisions – Data Transfer

Solutions: our own file format:

- assure valid & complete content of files
 - no interference with other parties
- add arbitrary user fields, files → analysis

db/cmr-files

extra information:

- version information of used code
- version information of CMR plug-ins (converter)
- version of db-file

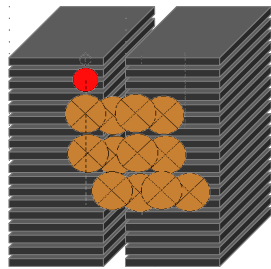
more advantages:

- create templates (chemisorption template: field: e_chem)
- data exchange

Decisions - Interfaces

Interfaces

- Accessible
- Programmable



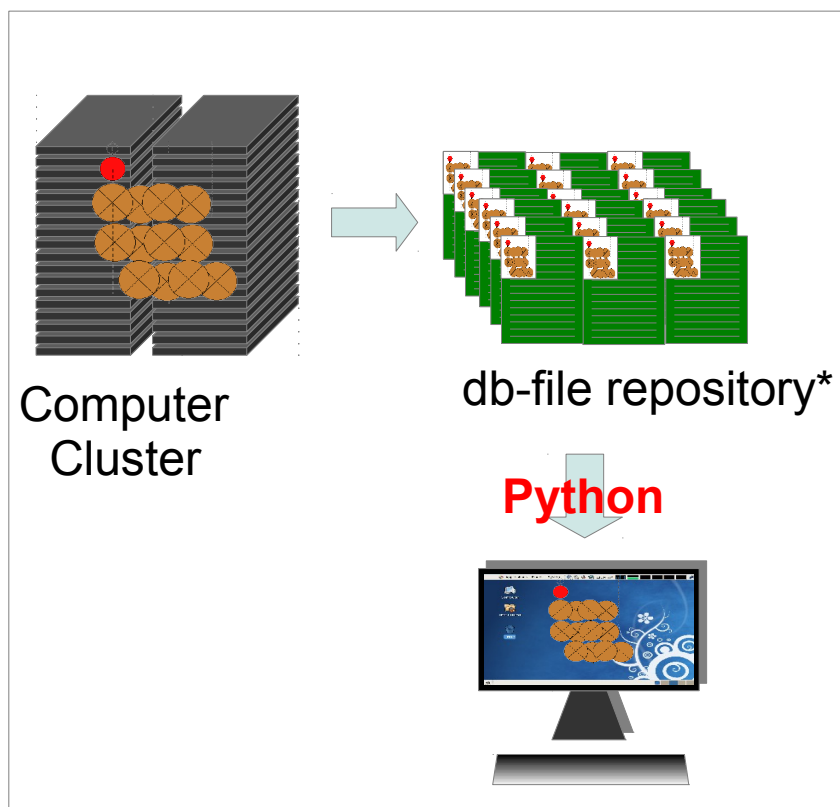
Computer Cluster

A screenshot of a web browser window displaying the 'Computational Materials Repository' interface. The browser's address bar shows 'http://localhost:8181/c' and the page title is 'Computational Materials R...'. The interface has a header with the title 'Computational Materials Repository' and a link to 'Modify query'. Below this is a navigation bar with five tabs: '1. Data set', '2. DB-Filters', '3. Enhancement', '4. Filters', and '5. Visualization'. Under the '1. Data set' tab, there are two sub-tabs: '1a. Default' and '1b. LP'. The main content area contains a text block explaining the query system: 'The data in this database is selected by writing queries into the field below. To make writing queries simpler, you can use the tabs above which are numbered 1-5. The tab row below shows subtabs e.g. "1a Default", "1b. LP". Click on the individual tabs to get more information about what they do. Generally it's good practise to start by restricting to data of a specific user e. g. db_user=dlandis. In order to see what users exist switch to tab "2. DB-Filters" to select user and keywords.' Below this is a 'Query:' section with a hint: '(Hint 1: use * to search for partial keywords; Hint 2: use " for keyword with spaces)'. There is a large text input field for the query. Below the input field is a 'Results per page:' dropdown menu set to '10'. At the bottom, there is an 'Execute' button and a link to 'or get result as' followed by icons for 'CMR' and 'json'. The bottom right corner shows 'Visitors: 1'.

Decisions - Interfaces

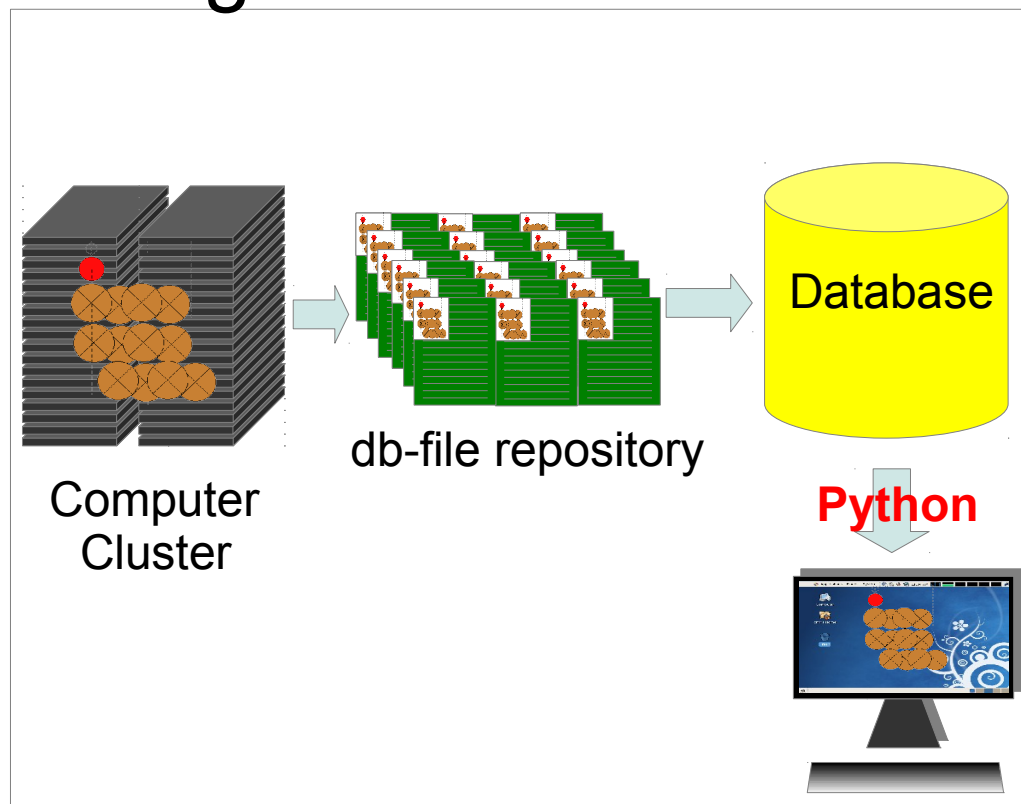
On Laptop:

- Programmable interface



On desktop computer with a database:

- Programmable interface



How to work with CMR

It's not a file-system:

- no file names
- no directories

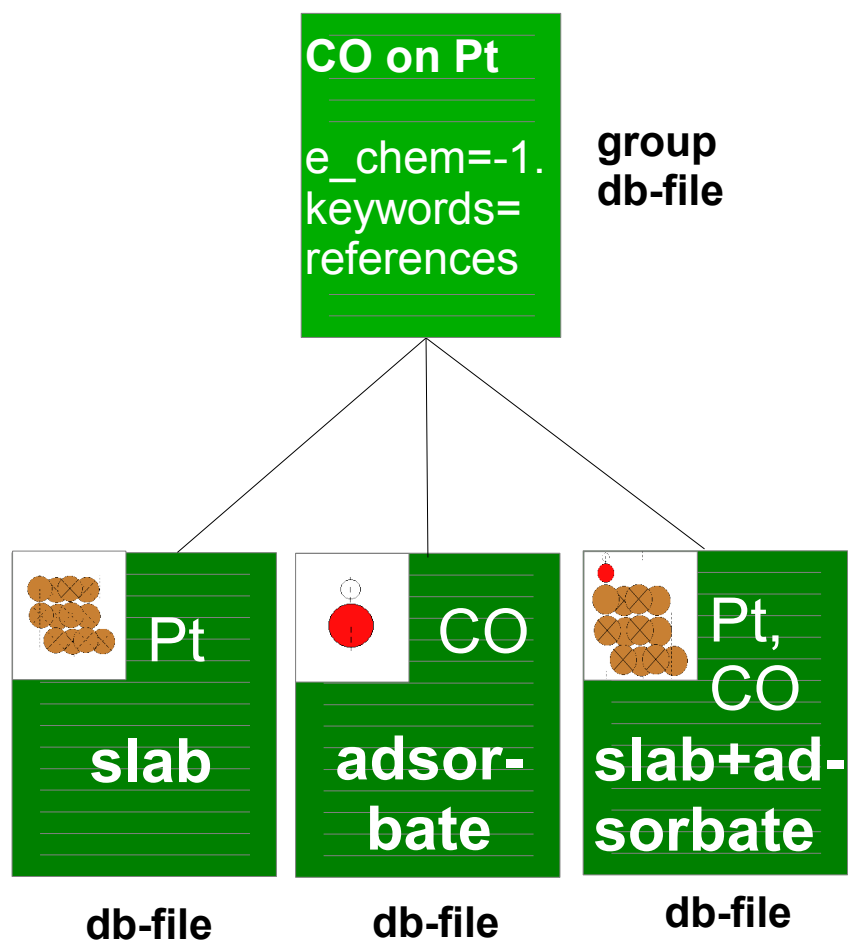
(actually there are *3DJEN832HNN129...cmr*)

How to work with CMR

- keyword
e.g. project_id, adsorption,
→ **find/identify** data quickly
- fields
e.g. adsorbate=CO, slab=Pt
→ provide more information/**combine** calculations
- groups
show how things belong together
→

Traceable Results

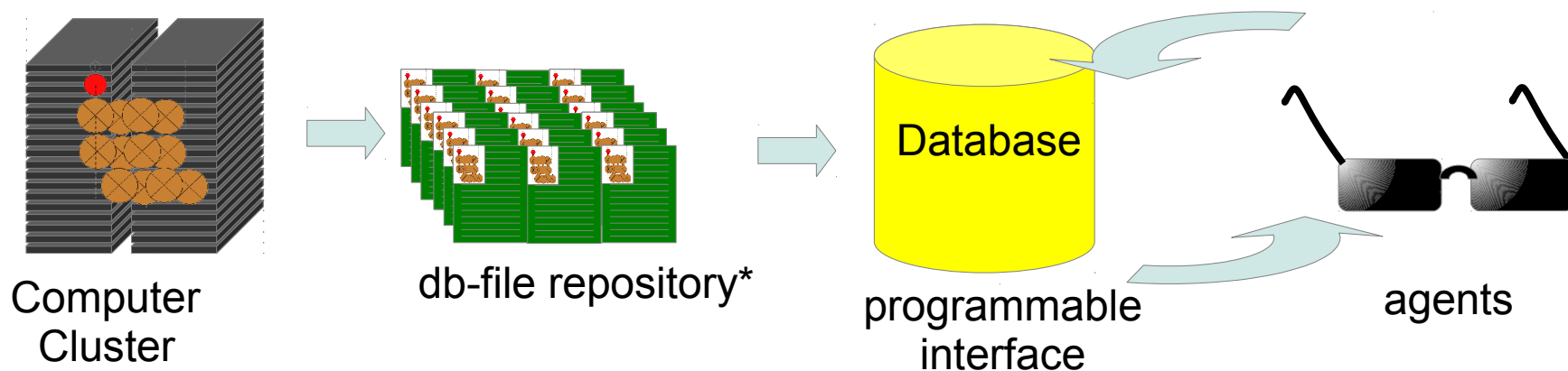
Show how things were calculated:



Agents (python)

Agent:

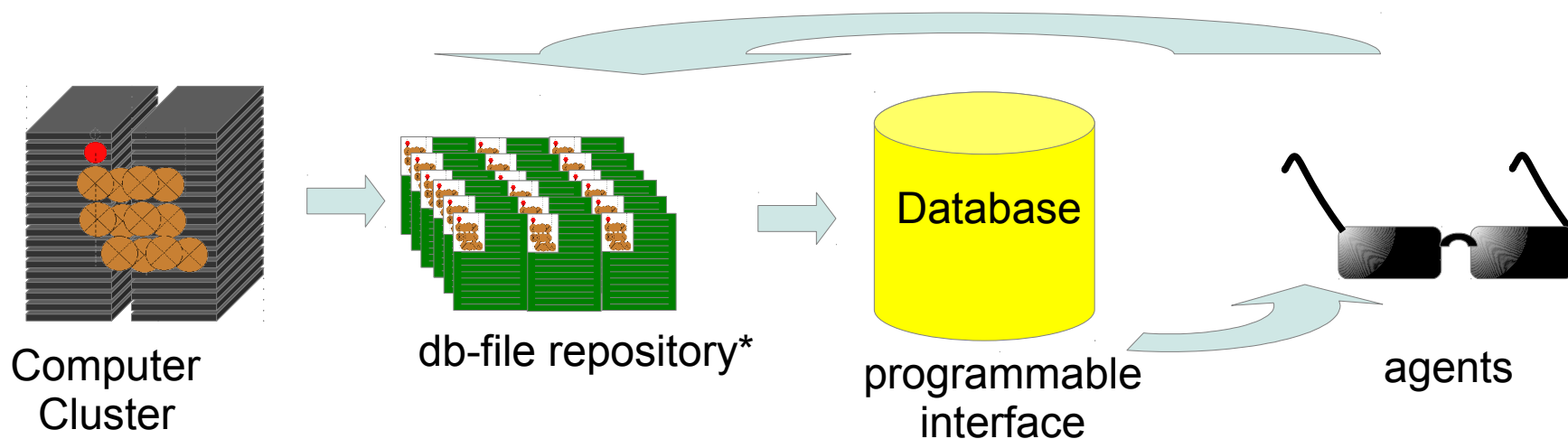
A (background) process that queries the database for certain keywords, and then groups calculations accordingly and performs operations (add, subtract etc.).



Agents (python)

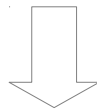
Agents:

Can be run as users as well, but cannot write directly to the database.



Grouping Agent

id	ads	site	slab	surface	energy	db_keywords
X 122	OH				...	[adsorbate]
Y 9			Ag	fcc111	...	[slab]
17			Ni	fcc111	...	[slab]
Z 18	OH	bridge	Ag	fcc111	...	[slab+adsorbate]
21	OH	fcc	Ag	fcc111	...	[slab+adsorbate]



id	ads	site	slab	surface	energy	references
2405	OH	bridge	Ag	fcc111	...	9, 18, 122

Criteria:

X.ads=Z.ads

Y.slab=Z.slab

Y.surf'=Z.surf'

Criteria are
customizable!

Querying

Web interface:

- shows what is there: results, groups, keywords, fields, scripts
- some analysis
- field restrictions
- read-only access
- download script for python – interface
- UI helps to create an intuitive query
- example later in case studies

The screenshot shows a web browser window with the address bar displaying `http://localhost:8181/c`. The page title is "Computational Materials Repository". Below the title, there is a "Modify query" link. The main content area is a form with five tabs: "1. Data set", "2. DB-Filters", "3. Enhancement", "4. Filters", and "5. Visualization". Under the "1. Data set" tab, there are two sub-tabs: "1a. Default" and "1b. LP". A text box contains instructions: "The data in this database is selected by writing queries into the field below. To make writing queries simpler, you can use the tabs above which are numbered 1-5. The tab row below shows subtabs e.g. '1a Default', '1b. LP'. Click on the individual tabs to get more information about what they do. Generally it's good practise to start by restricting to data of a specific user e. g. `db_user=dlandis`. In order to see what users exist switch to tab '2. DB-Filters' to select user and keywords." Below this, there is a "Query:" label with hints: "(Hint 1: use * to search for partial keywords; Hint 2: use \" for keyword with spaces)". A text input field contains the query: `adsorption atoms=Pt db_user=dlandis`. Below the input field, there is a "Results per page:" dropdown set to "10". At the bottom, there is an "Execute" button and a label "or get result as" followed by radio buttons for "JSON" and "JSON". The bottom right corner of the page shows "Visitors: 1".

Querying

Python user interface

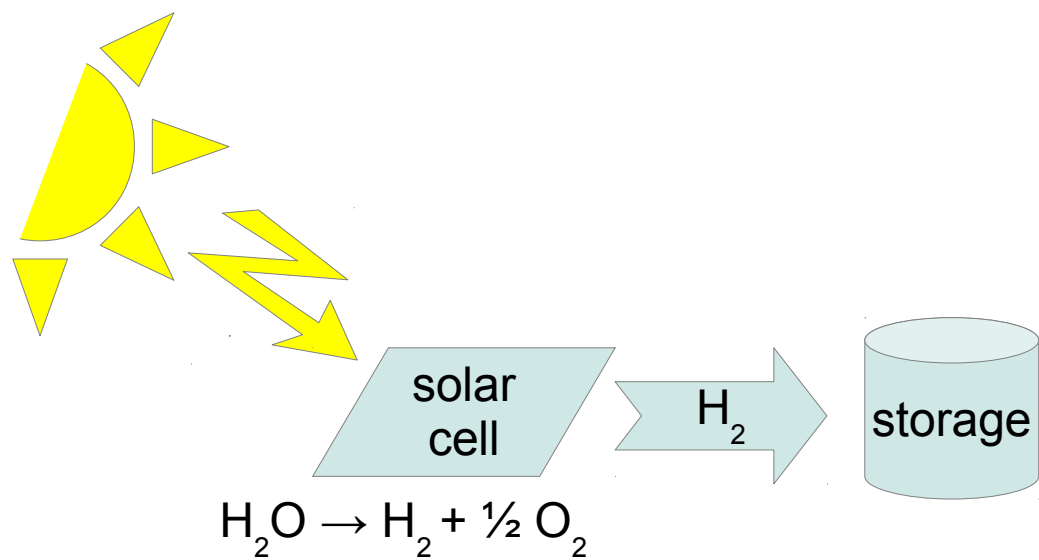
- create db/cmr-files
- query for keywords, fields & atoms
- access different databases
- modify database content
- run (user-) agents
- code example later in case studies

Supported Programs

- GPAW *
- VASP
- Gaussian
- Dacapo *
- ASE atoms *

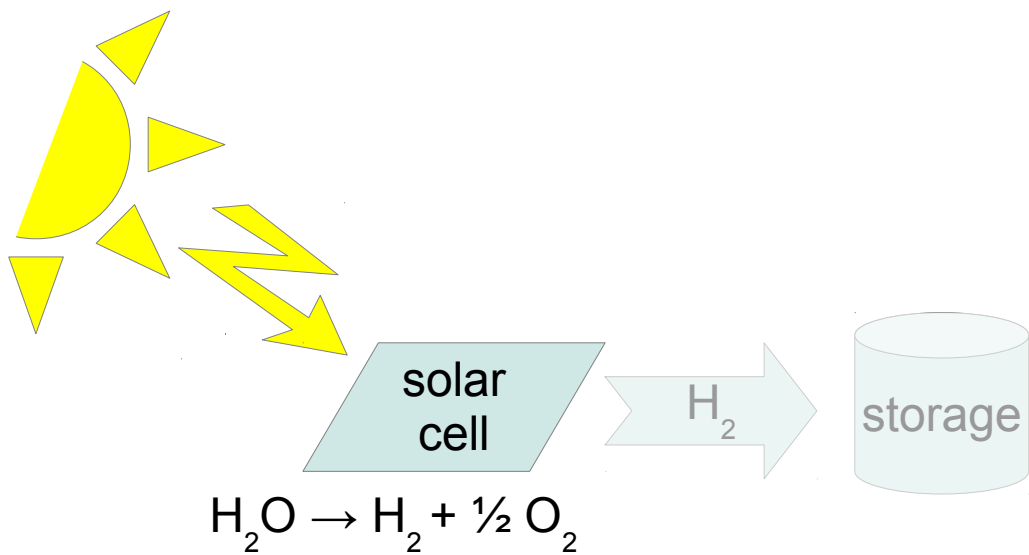
- CSV (spreadsheet) data

* In order to create db-files you need to have these programs installed. To read the created db-files you only need CMR.



Case Studies Overview

- Perovskite materials for optimal light capture
- Borohydride for hydrogen storage

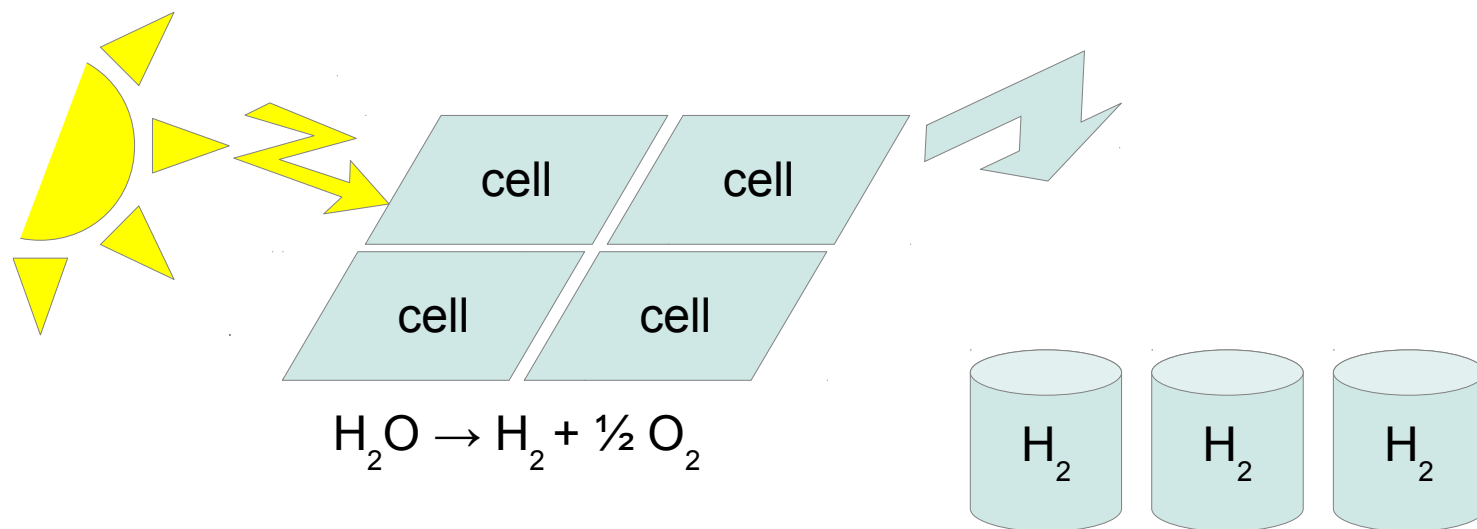


Computational Screening of Perovskite Metal Oxides for Optimal Solar Light Capture

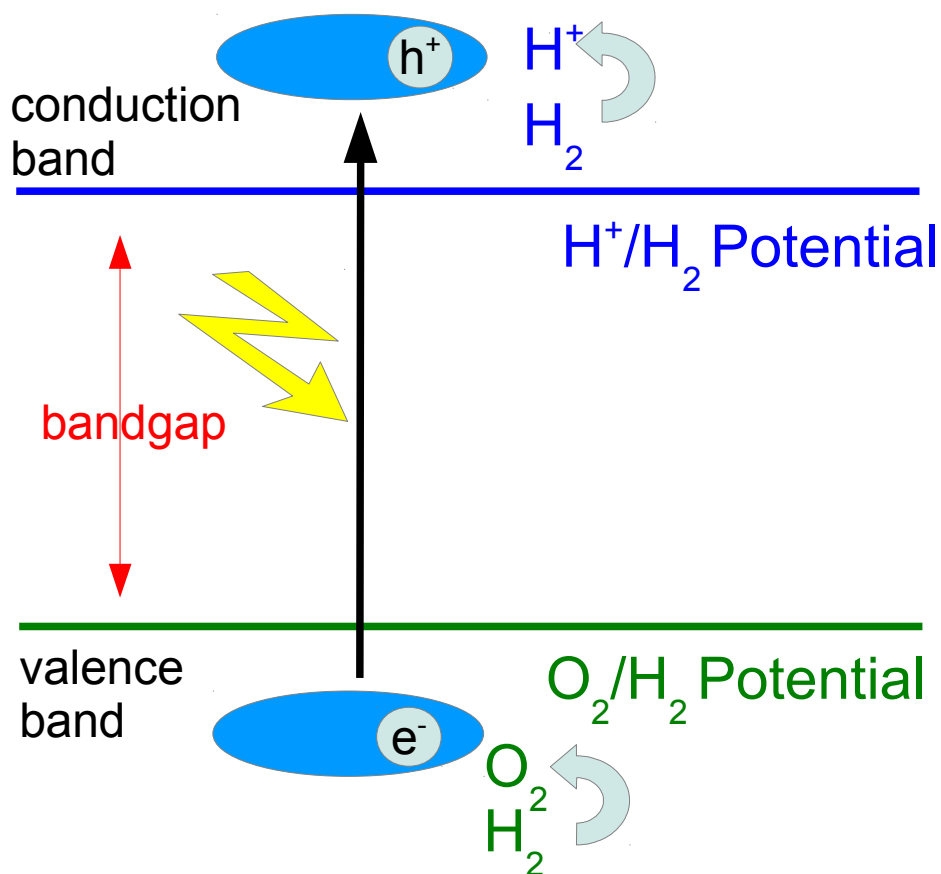
I. E. Castelli, T. Olsen, S. Datta, D. D. Landis, K. S. Thygesen, S. Dahl, K. W. Jacobsen
Energy Environ. Sci., vol. 5, 2012

Solar Cells

Photocatalytic cells → e.g. H_2



Water Splitting



derived from I.E. Castelli, CAMD, DTU Physics

Challenges:

- bandgap $> 1.23\text{eV} + \sim .25\text{eV}$
($H_2O \rightarrow H_2 + \frac{1}{2} O_2$)
- bottom conduction band more neg. t. reduction H^+/H_2
- top valence more pos. t. oxid' $O_2/H_2O/$
 $\rightarrow 1.5\text{eV} < \text{bandgap} < 3\text{eV}$
- stable material

Stability

The heat of formation was calculated with a **linear programming** algorithm:

$$\Delta E = \text{ABO}_3(\text{s}) - \min_{c_i} (c_1 \text{A}(\text{s}) + c_2 \text{B}(\text{s}) + c_3 \text{A}_x \text{O}_y(\text{s}) + c_4 \text{B}_x \text{O}_y(\text{s}) + c_5 \text{O})$$

bulk references
AO references
O reference

$c_1 + c_3 = 1$,
 $c_2 + c_4 = 1$,
 $c_3 + c_4 + c_5 = 3$

Data Set


H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

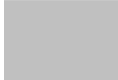
Screening of candidates:

- **52** different **elements**;
- Different **anions** (O, N);

AB + (O₃, O₂N) = 5400 combinations

Excluded elements:

 radio active, toxic

 non-metals

Analysis with CMR

1. Identify and enhance data

For ABO_3 and ABO_2N add field

combination=ABO3, resp. combination=ABO2N

A=Ba

B=Ta

conduction band=2.0

valence band=1.9

dir-gap=2

indir-gap=2

2. Identify reference (set)

e.g. $\text{Al}_{12}\text{O}_{18}$

composition=AO

keywords=references

1. Data set

2. DB-Filters

3. Enhancement

4. Filters

5. Visualization

1a. Default

1b. LP

Calculates the heat of formation using linear programming:

1. **Query for data** is the query for the compounds (e.g. "db_user=ivca").

2. **Select the data set:** Press "show available data sets" to show the available data set and select one (identified by the field "combination").

3. **Query for references** is the query that identified the references (e.g. "db_user=ivca references").

4. **Select subset of references:** Press "show available reference sets" to show the available references (identified by the field "composition").

Query for data:

db_user=ivca

Chose a data set:

ABO3 (2704)

show available data sets

Query for references:

references 10.1039/C1EE02717D

Chose reference sets:

show available reference sets

Add LP to query

It is recommended to show the following columns:

id_ref,A,B,anion,heat_of_formation,gllbsc_dir-ga

Add column selection



Query:

(Hint 1: use * to search for partial keywords; Hint 2: use " for keyword with spaces)

```
lin_prog="composition=ABN,ABO,AN,AO,AON,default,mbulk;
data_query=db_user=ivca;ref_query=references 10.1039/C1EE02717D;
combination=ABO3" jmol="width=100;height=100"
```

Results per page: 10

Execute

or get result as  or 





All ABO₃ with Heats of Formation

related
keywords

Restrict keywords:

- [O3 ±\(2704\)](#)
- [mox ±\(2704\)](#)
- [10.1039/C1EE02717D ±\(2704\)](#)
- [perovskite ±\(2704\)](#)
- [Q ±\(2704\)](#)
- [ABO3 ±\(2704\)](#)
- [Re ±\(103\)](#)
- [As ±\(103\)](#)
- [Sr ±\(103\)](#)
- [Rb ±\(103\)](#)
- [Cu ±\(103\)](#)





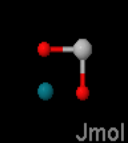















Download information:

-  a python script that retrieves this item from the database and creates an ase atoms object
-  a csv spread sheet with all the data
-  a python script that retrieves this item from the database
-  all the data in json format

Found 2704 results (0.470712s)

Fields

« 1 2 3 4 5 ... 271 »

id_ref	jmol	A	B	anion	heat_of_formation	gllbsc_dir-gap	gllbsc_ind-gap	CB_dir	CB_ind	VB_dir	VB_ind	atoms	db_keywords	doi	ingredients	downloads
8926		Rh	Re	O3	1.0400	0	0	5.9347	5.9347	5.9347	5.9347	O Rh Re (30, 1Rh, 1Re)	10.1039/C1EE02717D ABO3 mox Q O3 perovskite Re Rh RhReO3	10.1039/C1EE02717D	0.50 Re2 + 0.25 Rh4 + 3.00 O	  
8935		Rh	Ag	O3	2.3700	0	0	6.0569	6.0569	6.0569	6.0569	O Rh Ag (30, 1Rh, 1Ag)	10.1039/C1EE02717D ABO3 Ag mox Q O3 perovskite Rh RhAgO3	10.1039/C1EE02717D	0.25 Rh4 + 3.00 O + 0.25 Ag4	  
8938		Rh	Co	O3	1.5200	0	0	6.0182	6.0182	6.0182	6.0182	O Co Rh (30, 1Co, 1Rh)	10.1039/C1EE02717D ABO3 Co mox Q O3 perovskite Rh RhCoO3	10.1039/C1EE02717D	0.50 Co2 + 0.25 Rh4 + 3.00 O	  
8945		Rh	Cu	O3	1.9100	0	0	6.0677	6.0677	6.0677	6.0677	O Cu Rh (30, 1Cu, 1Rh)	10.1039/C1EE02717D ABO3 Cu mox Q O3 perovskite Rh RhCuO3	10.1039/C1EE02717D	0.25 Rh4 + 3.00 O + 0.25 Cu4	  
8946		Rh	Si	O3	1.1400	0	0	6.1417	6.1417	6.1417	6.1417	O Si Rh (30, 1Si, 1Rh)	10.1039/C1EE02717D ABO3 mox Q O3 perovskite Rh RhSiO3 Si	10.1039/C1EE02717D	0.25 O8Si4 + 0.25 Rh4 + 1.00 O	  

keywords

atoms

Publishing



**COMPUTATIONAL
MATERIALS
REPOSITORY**



Organisations:

[CAMD](#)
[DTU](#)

Collaboration:

[QMIP](#)

Software:

[ASE](#)
[GPAW](#)
[CMR](#)
[CAMPOS](#)

Public data sets:

Public CMR database	View the public database with published data
2012-02-22 Tandem cells etc.	Stability and bandgap screening; Tandem cells Ivano, in progress ...
2012-03-12 Reversible H storage	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project DOI:10.1063/1.3148892
2011-11-20 Stability and band gaps	Stability and bandgap screening Browse Stability and bandgap screening of 5400 compounds for new materials for solar light driven photo-electrocatalytic water splitting. DOI:10.1039/C1EE02717D

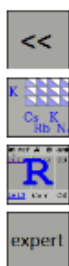
Publishing

go back

heat-map

references

query



[Hide search box](#)

Chose a data set: ABO3 (2704)
Reference electrode: NHE (-4.5 eV)
Keywords:
☒ Show atomic structure

Restriction 1:	heat_of_formation (eV)	≤	0.2
Restriction 2:	gllbsc_dir-gap (eV)	≥	1.5
Restriction 3:	gllbsc_dir-gap (eV)	≤	3
Restriction 4:		<	
Restriction 5:	heat_of_formation (eV)	<	
Restriction 6:	gllbsc_dir-gap (eV)	<	
Restriction 7:	gllbsc_ind-gap (eV)	<	
Restriction 8:	ase_total_energy (eV)	<	
	CB_dir	<	
	CB_ind	<	
	VB_dir	<	
	VB_ind	<	

Update

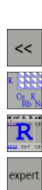
References:
☒ ABN (3)
☒ ABO (20)
☒ AN (50)
☒ AO (52)
☒ AON (35)
☒ default (3)
☒ mbulk (52)

Produces
query:

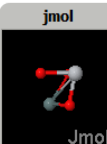









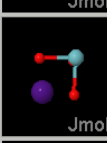



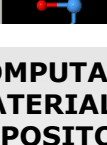

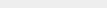

```
lin_prog="composition=ABN,ABO,AN,AO,AON,default,mbulk;data_query=db_user=ivca;ref_query=references
10.1039/C1EE02717D;combination=ABO3" columns=id_ref,jmol,A,B,anion,heat_of_formation,gllbsc_dir-
gap,gllbsc_ind-gap,CB_dir,CB_ind,VB_dir,VB_ind,atoms,db_keywords,doi,ingredients,downloads
jmol="width=100;height=100"
```

Publishing

Computational Materials Repository



± «1»

jmol	id_ref	A	B	anion	heat_of_formation	gllbse_dir-gap	gllbse_ind-gap	CB_dir	CB_ind	VB_dir	VB_ind	atoms	db_keywords	doi	ingredients	db_description	downloads
	9456	Sn	Ti	O3	0.1000	2.7000	2.5000	-0.0962	0.0188	2.6138	2.4988	O Ti Sn (30, 1Ti, 1Sn)	10.1039/C1EE02717D ABO3 mox Q O3 perovskite Sn SnTiO3 Ti	10.1039/C1EE02717D	0.12 Sn8 + 0.50 O4Ti2 + 1.00 O	Screening cubic perovskite structures, metal oxides	
	10760	Ca	Ge	O3	0.1600	2.7000	2.1000	-0.5353	-0.1953	2.2047	1.8647	Ge Ca O (1Ge, 1Ca, 3O)	10.1039/C1EE02717D ABO3 Ca CaGeO3 Ge mox Q O3 perovskite	10.1039/C1EE02717D	0.17 Ca6Ge6O18 + 0.00 Ge8	Screening cubic perovskite structures, metal oxides	
	10923	Li	V	O3	0.1700	2.1000	1.3000	-0.1168	0.2382	1.9332	1.5782	V O Li (1V, 3O, 1Li)	10.1039/C1EE02717D ABO3 Li LiVO3 mox Q O3 perovskite V	10.1039/C1EE02717D	0.06 O20V12 + 0.17 Li6O8V2 + 0.56 O	Screening cubic perovskite structures, metal oxides	
	10999	Sr	Ge	O3	0.1600	1.7000	1.2000	-0.1160	0.1140	1.5840	1.3540	Sr Ge O (1Sr, 1Ge, 3O)	10.1039/C1EE02717D ABO3 Ge mox Q O3 perovskite Sr SrGeO3	10.1039/C1EE02717D	0.08 Ge12O36Sr12	Screening cubic perovskite structures, metal oxides	
	11169	Na	V	O3	0.1000	1.7000	1	0.0094	0.3494	1.6894	1.3494	V Na O (1V, 1Na, 3O)	10.1039/C1EE02717D ABO3 mox Na NaVO3 Q O3 perovskite V	10.1039/C1EE02717D	0.12 Na8O24V8 + 0.00 Na8O4 + 0.00 V2	Screening cubic perovskite structures, metal oxides	
	11239	Ba	Sn	O3	-0.0800	2.5000	2.5000	-0.2948	-0.2948	2.2452	2.2452	Ba Sn O (1Ba, 1Sn, 3O)	10.1039/C1EE02717D ABO3 Ba BaSnO3 mox Q O3 perovskite Sn	10.1039/C1EE02717D	0.25 Ba4O4 + 2.00 O + 0.12 Sn8	Screening cubic perovskite structures, metal oxides	
	19450	Cs	Nb	O3	0.1800	2.9000	2.9000	-0.7520	-0.7420	2.1180	2.1080	Cs Nb O (1Cs, 1Nb, 3O)	10.1039/C1EE02717D ABO3 Cs CsNbO3 mox Nb Q O3 perovskite	10.1039/C1EE02717D	0.12 Cs8Nb8O24	Screening cubic perovskite structures, metal oxides	
	20605	Ga	Ta	O3	-0.0300	2.2000	2.1000	0.0391	0.0691	2.1991	2.1691	Ta Ga O (1Ta, 1Ga, 3O)	10.1039/C1EE02717D ABO3 Ga GaTaO3 mox Q O3 perovskite Ta	10.1039/C1EE02717D	0.38 Ga2O8Ta2 + 0.03 Ga8 + 0.12 Ta2	Screening cubic perovskite structures, metal oxides	
	20865	Ti	Ta	O3	0.1000	2	2	0.7396	0.7396	2.7796	2.7796	O Ta Ti (3O, 1Ta, 1Ti)	10.1039/C1EE02717D ABO3 mox Q O3 perovskite Ta Ti TiTaO3	10.1039/C1EE02717D	0.25 O12Ta4Ti4	Screening cubic perovskite structures, metal oxides	

Publishing

Computational Materials Repository

[Hide search box](#)

Do not forget to press **update matrix** after changing the selection!
If there is an error - it means that the dataset is already being calculated! Please wait a moments and try again.

Chose a data set: ABO3 (2704)

Width: 800

Height: 1200

X axis ticks: B

Y axis ticks: automatically selected

X sort order: Electronegativity (Paulin)

Y sort order: Electronegativity (Paulin)

Action on Click: show band edges

References:
☒ ABN (3)
☒ ABO (20)
☒ AN (50)
☒ AO (52)
☒ AON (35)
☒ default (3)
☒ mbulk (52)

	Value field:	Colors:
Triangle 1: (top-right)	gllbsc_ind-gap (eV)	0->white,0.7->purple,2.2->red
Triangle 2: (bottom-left)	heat_of_formation (eV)	min->red,0.3->white,4->blue
Triangle 3:		
Triangle 4:		

Examples for the **color** choice:

0->white,1->red,7->blue

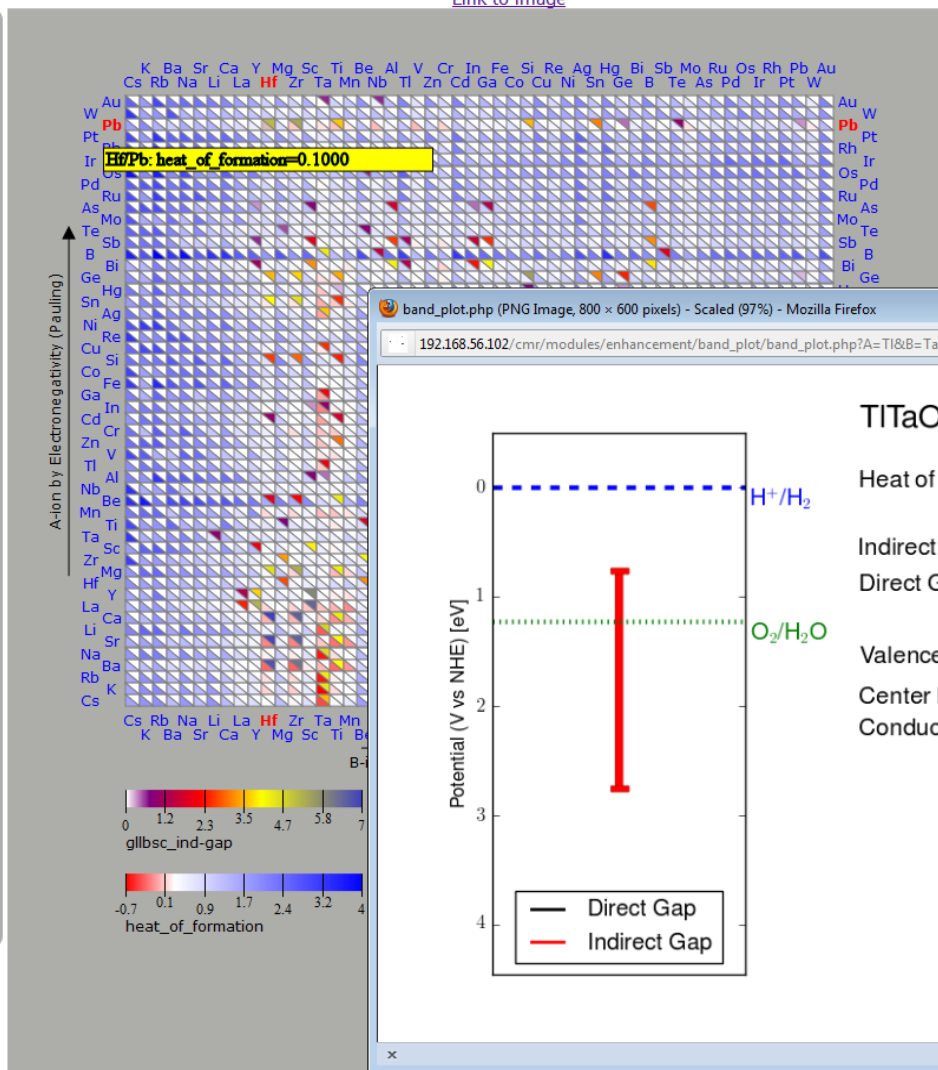
0->white,0.9->red,2.2->green,4->yellow,8->blue

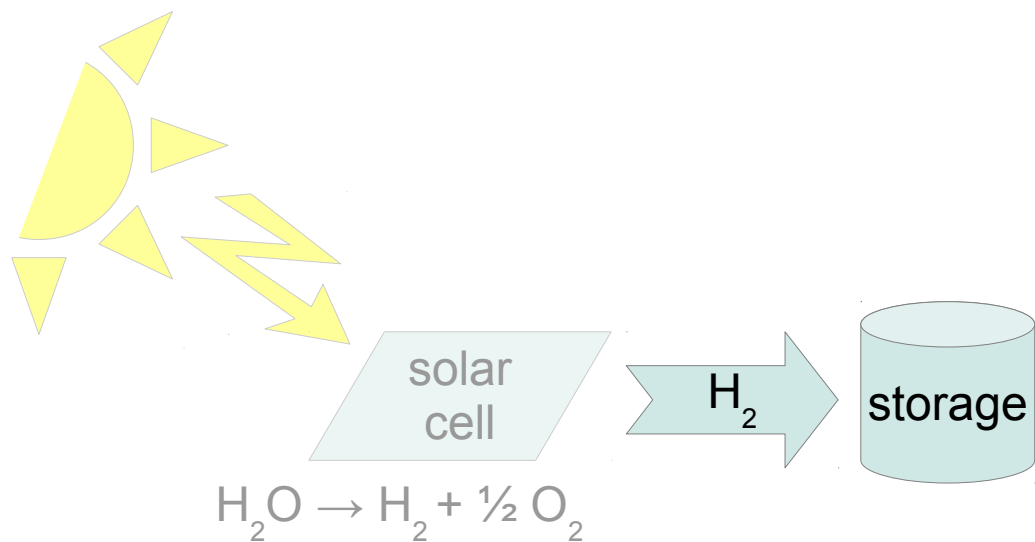
-100->blue,100->red

Valid color names are black, blue, cyan, green, gray, green, lightblue, pink, red, purple, white, yellow. Please note that the values must be in **increasing** order.

[Update matrix](#)

[Link to image](#)





Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project

Hummelshj, J. S. and Landis, D. D. et. al.
J. Chem. Phys., vol. 131, 2009

Aim:

Find candidates for hydrogen storage *for further investigation.*

Hydrogen Storage

What we investigated:

Borohydrides:

- $M_1 M_2 (BH_4)_x$ with $x=2,3,4,5$
- $M_1 = \{\text{Li, Na, K}\}$ (orange) $M_2 = \{\text{alk. alk earth, 3d, 4d metals}\}$ (yellow)
- different structures (see paper)

Hydrogen Storage

What we investigated:

- stability against phase separation

$$\Delta E_{\text{alloy}} = E_{\text{LiSc}(\text{BH}_4)_4} - (E_{\text{Li}(\text{BH})_4} + E_{\text{Sc}(\text{BH}_4)_3})$$

- decomposition (pathway)

$$\Delta E_{\text{decomp}} = E_{\text{LiMn}(\text{BH}_4)_3} - (E_{\text{LiH}} + E_{\text{Mn}} + 3 E_B + 5.5 E_{\text{H}_2})$$

Hydrogen Storage

What we investigated:

assessing stability:

- what is more stable

$$E_{LiSc(BH_4)_3} ? E_{LiSc(BH_4)_2}$$

- effective reference value:

$$E^*_{LiSc(BH_4)_2} = E_{LiSc(BH_4)_3} - 2 E_{H_2} - E_B$$

→ most stable structure, hydrogen density, weight percent

Hydrogen Storage with CMR

What needs to be done with CMR in order to be able to query:

- identify data with keywords and fields:
keywords: reference, calc, project id
fields: all values that need to be queried
alkali, metal, number of B atoms, weight %
- alloy energy, decomposition energy (→ references)
 1. add directly to db-file
 2. add extra (group) layer

Hydrogen Storage with CMR

References for alloy and decomposition energy:

db-file containing a dacapo calculation

$\text{KAg}(\text{BH}_4)_3$
total energy=-2665.1
weight %=12.1
structure=to

db-file containing a group calculation

$\text{KAg}(\text{BH}_4)_3$
total energy=-2665.1
weight %=12.1
structure=to
keywords=complete
allow_energy=...
decomp_energy=...

1st set of
reference energies

Ag
K
H4BAg
H4K4
H8K2B2

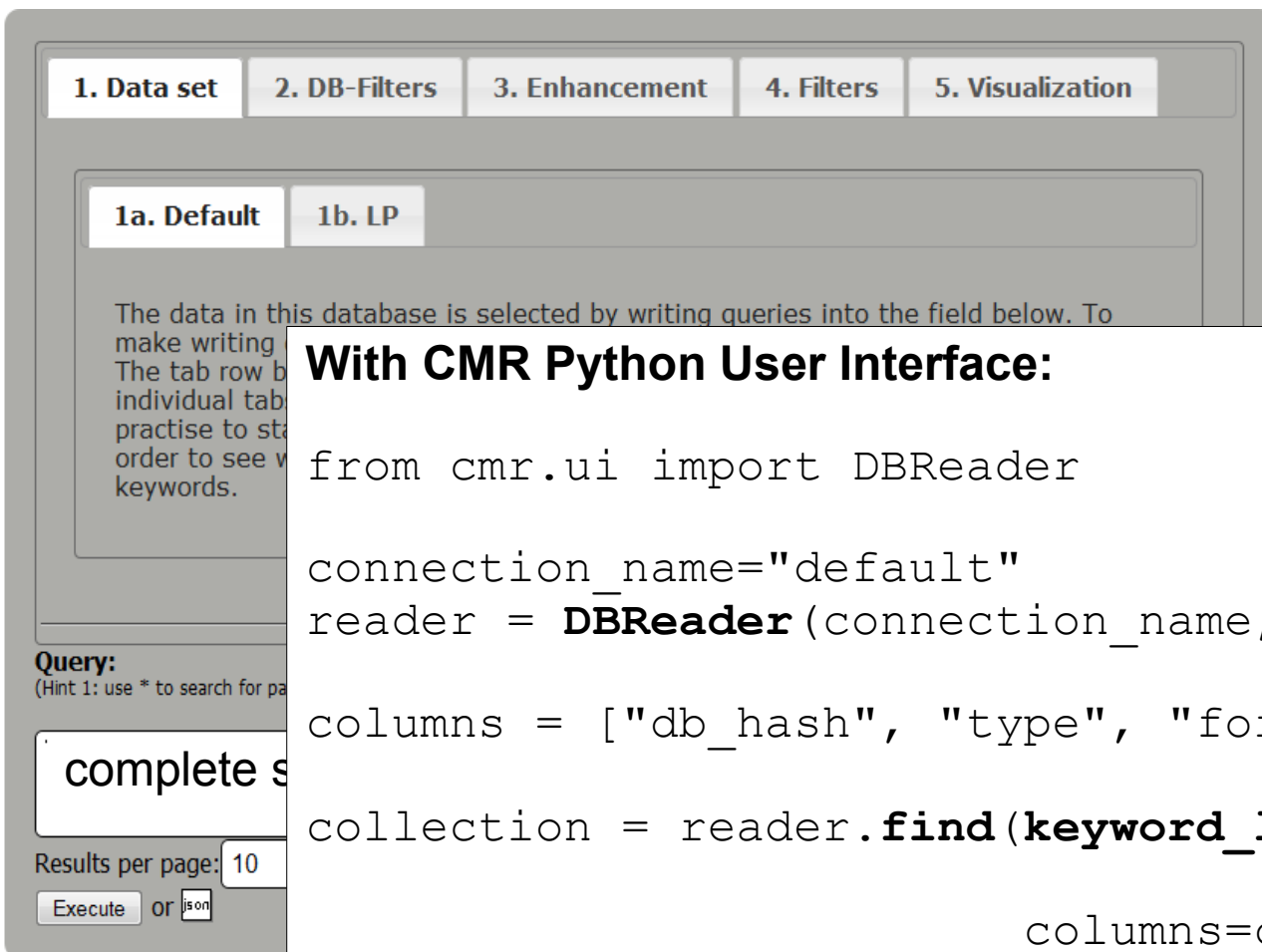
2nd set of
reference energies

Ag
K
H4BAg
H4K4
H8K2B2

references, so we know how
decomposition energy was
calculated

Hydrogen Storage with CMR

Querying for all structures:



With CMR Python User Interface:

```
from cmr.ui import DBReader

connection_name="default"
reader = DBReader(connection_name, db_prefix="aio")

columns = ["db_hash", "type", "formula", "structure", ...]

collection = reader.find(keyword_list=["complete",
                                       "school08"],
                        columns=columns)

collection.print_table(columns=columns)
```

Hydrogen Storage with CMR

1. Preferred alloy systems $M_1M_2(BH_4)_x$

1. Data set 2. DB-Filters 3. Enhancement 4. Filters 5. Visualization

The following filters will be applied just before visualizing the data. This means they will take longer, but they are able to handle calculated/enhanced columns as well.

4a. restriction filter 4b. Order 4c. Or 4d. select lowest

1st field:

2nd field:

3rd field:

Field to minimize:

Query:
(Hint 1: use * to search for partial keywords; Hint 2: use " for keyword with spaces)

Results per page:

or

Select lowest:

structure	type	formula	eff_energy
t	KAg	KAgB3H12	-2668.3
to	KAg	KAgB3H12	-2667.3
t	KAg	KAgB4H12	-2669.6

Hydrogen Storage with CMR

2. Best $M_1M_2(BH_4)_x$ with $\Delta E_{alloy} < 0$ and $\Delta E_{decomp} < 0$

1. Data set

2. DB-Filters

3. Enhancement

4. Filters

5. Visualization

The following filters will be applied just before visualizing the data. This means they will take longer, but they are able to handle calculated/enhanced columns as well.

4a. restriction filter

4b. Order

4c. Or

4d. select lowest

delta_E_

<

0

Add

Update available fields

Query:

(Hint 1: use * to search for partial keywords; Hint 2: use " for keyword with spaces)

school08 complete

sel_lowest="col1=type;min=effective_energy"

filter2="delta_E_decomp<0;delta_E_alloy<0;"

Execute

or

json

Hydrogen Storage with CMR

2. Best $M_1M_2(BH_4)_x$ with $\Delta E_{alloy} < 0$ and $\Delta E_{decomp} < 0$

With CMR Python User Interface:

```
1. from cmr.ui import DBReader

connection_name="default"
reader = DBReader(connection_name, db_prefix="aio")

columns = ["db_hash", "type", "formula", "structure", ...]

collection = reader.find(keyword_list=["complete",
                                     "school08"],
                        columns=columns)

collection.sort("type")
collection = collection.select_lowest("effective_energy")
collection.sort("delta_E_decomp")
collection.select("delta_E_decomp", 0, Operator("<"), True)

collection.sort("delta_E_alloy")
collection.select("delta_E_alloy", 0, Operator("<"), True)

collection.print_table(columns=columns)
```

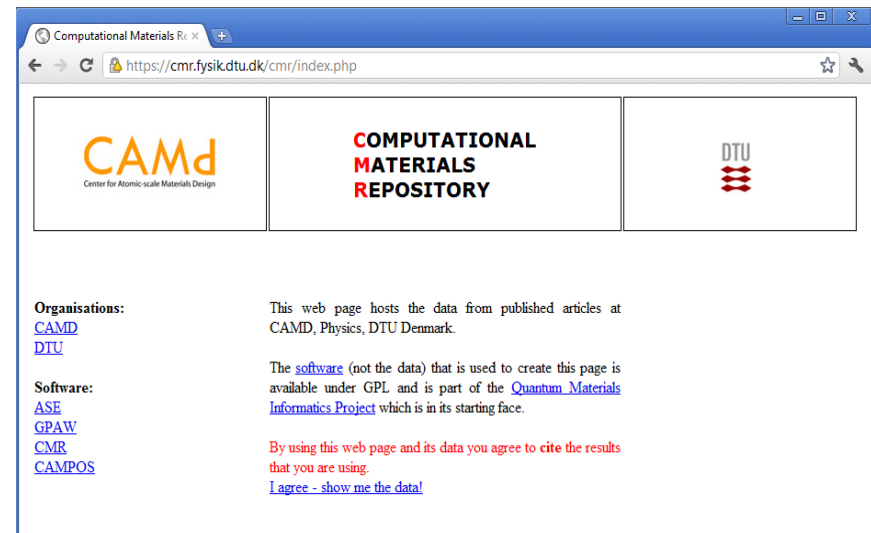
Summary

We have presented an open source database framework for electronic structure calculations that can be used for research.

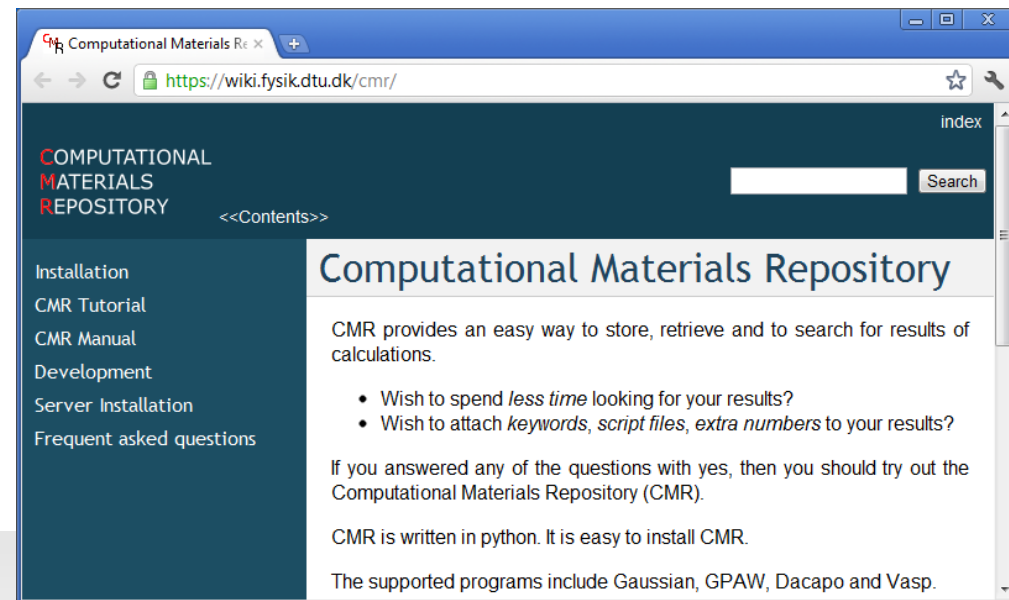
- collecting data from different codes
- different user interfaces
- analysis data
- data exchange/sharing
- publishing

Summary

- Accessible at
<http://cmr.fysik.dtu.dk>



- Install from
<http://wiki.fysik.dtu.dk/cmr>



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