

# Computational Materials Repository

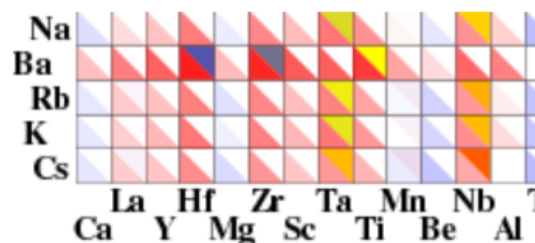
## User Manual

---

Center for Atomic-Scale Materials Design  
Department of Physics  
Technical University of Denmark



## Stability and bandgap screening of 5400 compounds for new materials for solar light driven photo- electrocatalytic water splitting.

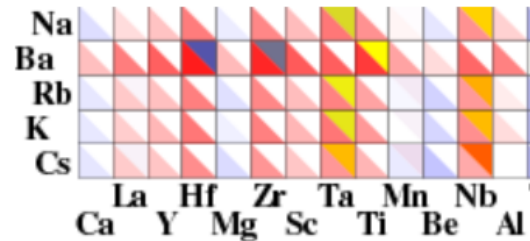


- [heat map](#)
- [search box](#)
- [manual](#)

For almost 40 years researchers have tried to identify semiconductors suitable for photo-electrochemical water splitting under solar light. Investigations have focused on oxides and, more recently on oxynitrides, due to their good properties with respect to stability. Inspired by this, we have performed a comprehensive computational screening of more than 5400

**Stability and bandgap screening of 5400 compounds  
for new materials for solar light driven photo-  
electrocatalytic water splitting.**

**Visual  
representation of  
selected  
properties for our  
sets of data**



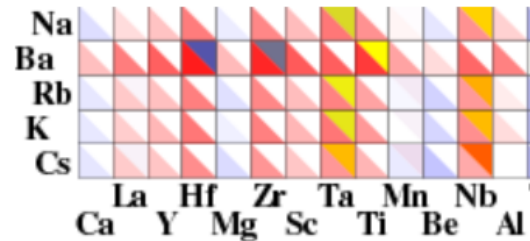
- [heat map](#)
- [search box](#)
- [manual](#)

For almost 40 years researchers have tried to identify semiconductors suitable for photo-electrochemical water splitting under solar light. Investigations have focused on oxides and, more recently on oxynitrides, due to their good properties with respect to stability. Inspired by this, we have performed a comprehensive computational screening of more than 5400



## Stability and bandgap screening of 5400 compounds for new materials for solar light driven photo- electrocatalytic water splitting.

Data view of our  
sets of data with  
restrictions on  
properties  
selected by the  
user

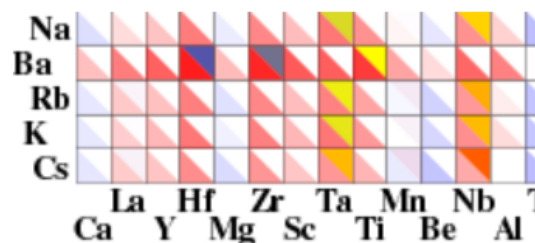


- [heat map](#)
- [search box](#)
- [manual](#)

For almost 40 years researchers have tried to identify semiconductors suitable for photo-electrochemical water splitting under solar light. Investigations have focused on oxides and, more recently on oxynitrides, due to their good properties with respect to stability. Inspired by this, we have performed a comprehensive computational screening of more than 5400



## Stability and bandgap screening of 5400 compounds for new materials for solar light driven photo- electrocatalytic water splitting.



Here you are!

- [heat map](#)
- [search box](#)
- [manual](#)

For almost 40 years researchers have tried to identify semiconductors suitable for photo-electrochemical water splitting under solar light. Investigations have focused on oxides and, more recently on oxynitrides, due to their good properties with respect to stability. Inspired by this, we have performed a comprehensive computational screening of more than 5400



Search box

## Computational Materials Repository

Heat map

[Hide search box](#)

>go to the data view interface<

Combination: ABO3

Action on Click: show band edges

X axis ticks: B

Y axis ticks: automatically selected

X sort order: Electronegativity (Paulir)

Y sort order: Electronegativity (Paulir)

Width: 800

Height: 1200

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

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

Examples for the color choice:

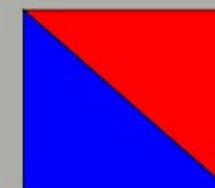
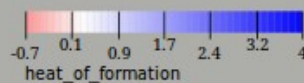
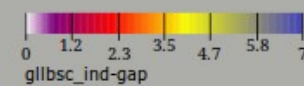
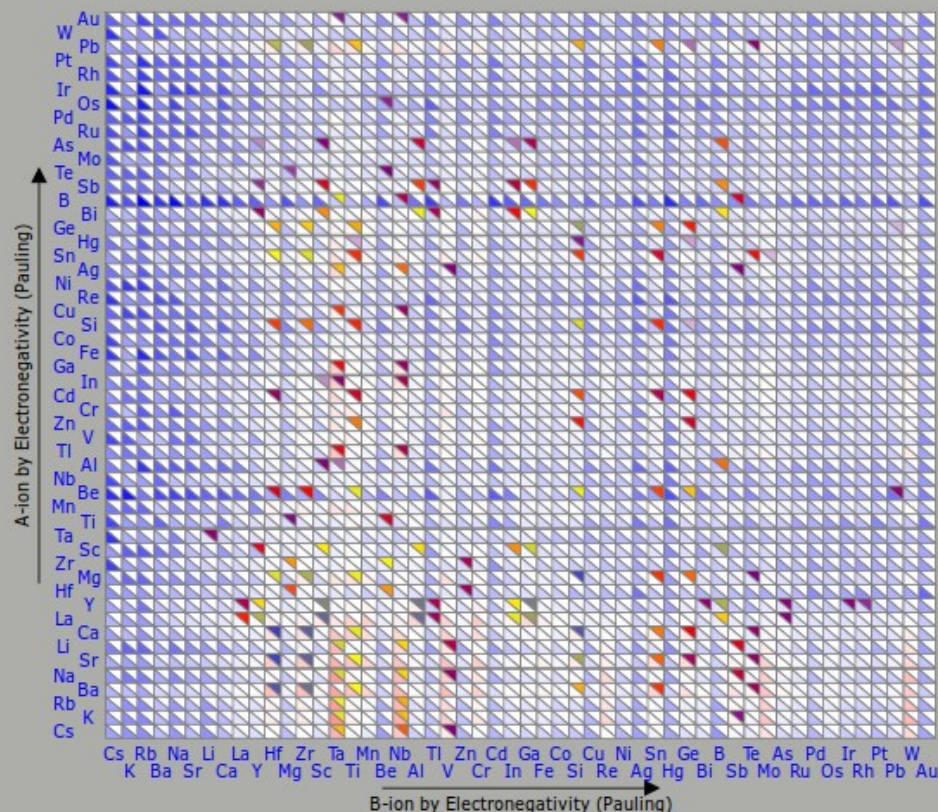
0->white,1->red,7->blue

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



> [go to the data view interface](#) <

Combination:  

Action on Click:

X axis ticks:

Y axis ticks:

X sort order:

Y sort order:

Width:

Height:

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

	Value field:	Colors:
Triangle 1: (top-right)	<input type="text" value="gllbse_ind-gap (eV)"/>	<input type="text" value="0-&gt;white,0.7-&gt;purple,2.2-&gt;re"/>
Triangle 2: (bottom-left)	<input type="text" value="heat_of_formation (eV)"/>	<input type="text" value="-2-&gt;red,0.3-&gt;white,4-&gt;blue"/>
Triangle 3:	<input type="text"/>	<input type="text"/>
Triangle 4:	<input type="text"/>	<input type="text"/>


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.



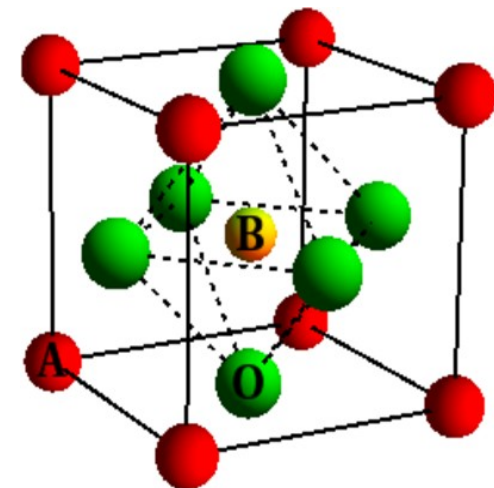
## Combination:

Chemical composition in the perovskite crystal structure;

Available sets:

- $\text{ABO}_3$ ;
- $\text{ABO}_2\text{N}$ .

Cubic perovskite structure:



Update the matrix!

> [go to the data view interface](#) <

Combination: ABO3  
Action on Click: show band edges  
X axis ticks: B  
Y axis ticks: automatically selected  
X sort order: Electronegativity (Pauli  
Y sort order: Electronegativity (Pauli

Width:  
800  
Height:  
1200

References:

☒ abn  
☒ abox  
☒ an  
☒ aox  
☒ aoxn  
☒ bulk

	Value field:	Colors:
Triangle 1: (top-right)	gllbsc_ind-gap (eV)	0->white,0.7->purple,2.2->re
Triangle 2: (bottom-left)	heat_of_formation (eV)	-2->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

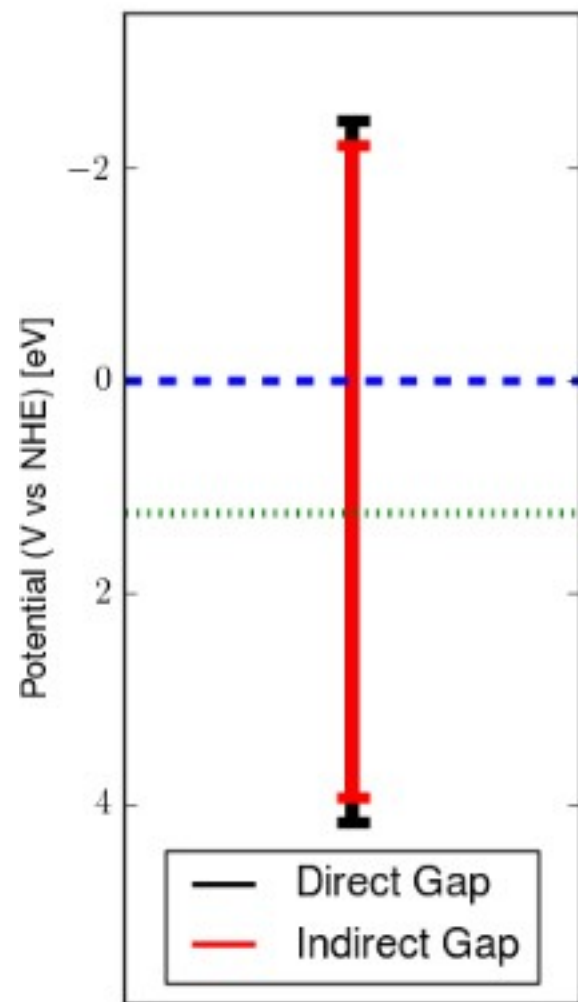
Valid color names are black, blue, cyan, green, gray, green, lightblue, pink, red, purple, white, yellow. Please note that the values must be in **increasing** order.

Update matrix

## Action on Click:

Band edges position or calculation data are available with a click on each small square in the heat map.





DOI: 10.1039/b000000x

$\text{YAlO}_3$

Heat of Form. = 0.14 eV/atom

Indirect Gap = 6.15 eV

Direct Gap = 6.62 eV

Valence Band = 3.9 (4.2) eV

Center Band = 0.8 eV

Conduction Band = -2.2 (-2.5) eV

**Show band edges:**

(in order of appearance)

Composition

Heat of Formation

Indirect Gap

Direct Gap

Band edges position  
for the indirect  
(direct) bandgap

DOI of the paper  
where this data has  
been published first




## Computational Materials Repository

Units: all variable names starting with "ase\_" are in eV and Angstrom. Other units are program/code specific.

Show calculation  
data:

All data available  
from the calculation

Download

id_ref	4896
downloads	  
group members	
member in group	
db_user	ivca
db_date	2011-11-09 10:17:48.743431
db_keywords	<a href="#">perovskite</a> <a href="#">mox</a> <a href="#">Al</a> <a href="#">O</a> <a href="#">ABO3</a> <a href="#">Y</a> <a href="#">O3</a> <a href="#">YAlO3</a>
A	Y
AluminiumFingerprint	b4fdb5400e294dfa8da7b1d19297efc9
anion	O3
architecture	x86_64
ase_atomic_numbers	[39, 13, 8, 8, 8]
ase_cell	[[3.7110105285299, 0, 0], [0, 3.7110105285299, 0], [0, 0, 3.7110105285299]]
ase_center_of_mass	[0.67533724196131, 0.66777254772375, 0.66777254772375]
ase_charges	[0, 0, 0, 0, 0]
ase_chemical_symbols	[Y, Al, O, O, O]
ase_dlr	/home/camp/ivca/ase/ase
ase_initial_magnetic_moments	[3.2624153208394E-5, -1.2823152270223E-5, 0.00017040569710692, -7.9652309964155E-5, -7.9700403992576E-5]
ase_kinetic_energy	0



Our calculations are performed using the Plane-waves DFT code

All the structures have been fully optimized using an RPBE functional [2];

For the evaluation of the bandgap, the GLLB-SC functional [3] has been used;

The heat of formation has been calculated using a linear programming algorithm with a vast pool of references. Oxygen has been taken at the chemical potential of water:

$$\Delta E = \text{ABO}_3(\text{s}) - \min_{c_i} (c_1 \text{A}(\text{s}) + c_2 \text{B}(\text{s}) + c_3 \text{A}_x \text{O}_y(\text{s}) + c_4 \text{B}_x \text{O}_y(\text{s}) + c_5 \text{O})$$
$$c_1 + c_3 = 1, \quad c_2 + c_4 = 1, \quad c_3 + c_4 + c_5 = 3$$

[2] J. Nørskov *et al.*, *Journal of Physical Chemistry B*, 2004, **108**, 17886-17892.

[3] O. Gritsenko *et al.*, *Journal of Physical Review A*, 1995, **51**, 1944.

## GLLB-SC Potential [3]:

GLLB: Gritsenko, van Leeuwen, van Lenthe and Baerends

SC: Solid and Correlation. Better description for solids.

GLLB:  $B_{88}$  and no correlation.

Screening potential

$$v_{\text{GLLB-SC}}(\mathbf{r}) = 2\epsilon_{\text{xc}}^{\text{PBEsol}}(\mathbf{r}) + \sum_i^{\text{occ}} K_x \sqrt{\epsilon_r - \epsilon_i} \frac{|\psi_i(\mathbf{r})|^2}{n(\mathbf{r})} + v_{\text{c,resp}}^{\text{PBEsol}}(\mathbf{r})$$

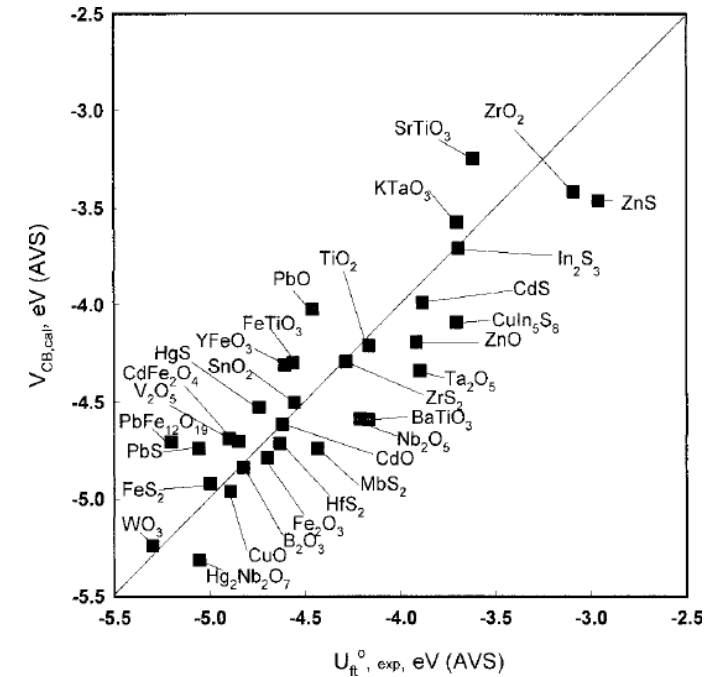
Exchange response: it contains the derivative discontinuity

The position of the band edges have been obtained using the empirical equation [4,5]:

$$E_C = (\chi_A \chi_B \chi_O^3)^{1/5} - 1/2 E_{gap} + E_0$$

Where:

- $\chi = 1/2 (A + I_1)$  is the absolute electronegativity (Mulliken scale);
- $A$  is the electron affinity;
- $I_1$  is the first ionization energy;
- $E_{gap}$  is the bandgap;
- $E_0$  is the reference electrode relative to vacuum.



[4] M.A. Butler *et al.*, *Journal of the Electrochemical Society*, 1978, **125**, 228-232.

[5] Y. Xu *et al.*, *American Mineralogist*, 2000, **85**, 543-556.

More detail of the method:

[6] I.E. Castelli, T. Olsen, S. Datta, D.D. Landis, K.S. Thygesen, S. Dahl, K.W. Jacobsen, *Energy & Environmental Science*, Supplementary Online Information, in printing.



>[go to the data view interface](#)<

Combination: ABO3  
Action on Click: show band edges  
X axis ticks: B  
Y axis ticks: automatically selected  
X sort order: Electronegativity (Pauli  
Y sort order: Electronegativity (Pauli

Width: 800  
Height: 1200

References:

☒ abn  
☒ abox  
☒ an  
☒ aox  
☒ aoxn  
☒ bulk

	Value field:	Colors:
Triangle 1: (top-right)	gllbse_ind-gap (eV)	0->white,0.7->purple,2.2->re
Triangle 2: (bottom-left)	heat_of_formation (eV)	-2->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

## X axis ticks:

A- and B- ion are not equivalent in the cubic perovskite structure. Select which of the two has to be shown along the X axis

> [go to the data view interface](#) <

Combination:

Action on Click:

X axis ticks:

Y axis ticks:

X sort order:

Y sort order:

Width:

Height:

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

	Value field:	Colors:
Triangle 1: (top-right)	<input type="text" value="gllbsc_ind-gap (eV)"/>	<input type="text" value="0-&gt;white,0.7-&gt;purple,2.2-&gt;re"/>
Triangle 2: (bottom-left)	<input type="text" value="heat_of_formation (eV)"/>	<input type="text" value="-2-&gt;red,0.3-&gt;white,4-&gt;blue"/>
Triangle 3:	<input type="text"/>	<input type="text"/>
Triangle 4:	<input type="text"/>	<input type="text"/>

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.

## X/Y sort order:

Different orders for the chemical elements are available:

- Alphabetical;
- Atomic number;
- Electronegativity;
- First Ionization Energy;
- Weight;
- Density;
- Abundance;
- Atomic Radii;
- Covalent Radii;
- Lowest possible oxidation number;
- Pettiform Map;
- Cost.

> [go to the data view interface](#) <

Combination:

Action on Click:

X axis ticks:

Y axis ticks:

X sort order:

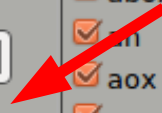
Y sort order:

Width:

Height:

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk



	Value field:	Colors:
Triangle 1: (top-right)	<input type="text" value="gllbse_ind-gap (eV)"/>	<input type="text" value="0-&gt;white,0.7-&gt;purple,2.2-&gt;re"/>
Triangle 2: (bottom-left)	<input type="text" value="heat_of_formation (eV)"/>	<input type="text" value="-2-&gt;red,0.3-&gt;white,4-&gt;blue"/>
Triangle 3:	<input type="text"/>	<input type="text"/>
Triangle 4:	<input type="text"/>	<input type="text"/>

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.

## Width/Height:

Width and Height of the heat map.

A square table correspond to 800\*1200

> [go to the data view interface](#) <

Combination:   
Action on Click:   
X axis ticks:   
Y axis ticks:   
X sort order:   
Y sort order:

Width:   
Height:

References:  
☒ abn  
☒ abox  
☒ an  
☒ aox  
☒ aoxn  
☒ bulk

	Value field:	Colors:
Triangle 1: (top-right)	<input type="text" value="gllbsc_ind-gap (eV)"/>	<input type="text" value="0-&gt;white,0.7-&gt;purple,2.2-&gt;re"/>
Triangle 2: (bottom-left)	<input type="text" value="heat_of_formation (eV)"/>	<input type="text" value="-2-&gt;red,0.3-&gt;white,4-&gt;blue"/>
Triangle 3:	<input type="text"/>	<input type="text"/>
Triangle 4:	<input type="text"/>	<input type="text"/>

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.

## References:

Combinations to include in the pool of references for the LINEAR PROGRAMMING algorithm used for the evaluation of the formation energy. Only the most stable structure for each combination has been included

> [go to the data view interface](#) <

Combination:

Action on Click:

X axis ticks:

Y axis ticks:

X sort order:

Y sort order:

Width:

Height:

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

	Value field:	Colors:
Triangle 1: (top-right)	<input type="text" value="gllbsc_ind-gap (eV)"/>	<input type="text" value="0-&gt;white,0.7-&gt;purple,2.2-&gt;re"/>
Triangle 2: (bottom-left)	<input type="text" value="heat_of_formation (eV)"/>	<input type="text" value="-2-&gt;red,0.3-&gt;white,4-&gt;blue"/>
Triangle 3:	<input type="text"/>	<input type="text"/>
Triangle 4:	<input type="text"/>	<input type="text"/>

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.

## Triangle #:

Each square in the pattern can be divided in up to 4 triangles with different properties:

- Heat of Formation;
- Indirect bandgap (GLLBSC ind-gap);
- Direct bandgap (GLLBSC dir-gap);
- ASE total energy.

Different color maps can be chosen by the user (default values as in [1])



>[go to the data view interface](#)<

Combination:

Action on Click:

X axis ticks:

Y axis ticks:

X sort order:

Y sort order:

Width:

Height:

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

	Value field:	Colors:
Triangle 1: (top-right)	<input type="text" value="gllbsc_ind-gap (eV)"/>	<input type="text" value="0-&gt;white,0.7-&gt;purple,2.2-&gt;re"/>
Triangle 2: (bottom-left)	<input type="text" value="heat_of_formation (eV)"/>	<input type="text" value="-2-&gt;red,0.3-&gt;white,4-&gt;blue"/>
Triangle 3:	<input type="text"/>	<input type="text"/>
Triangle 4:	<input type="text"/>	<input type="text"/>

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.

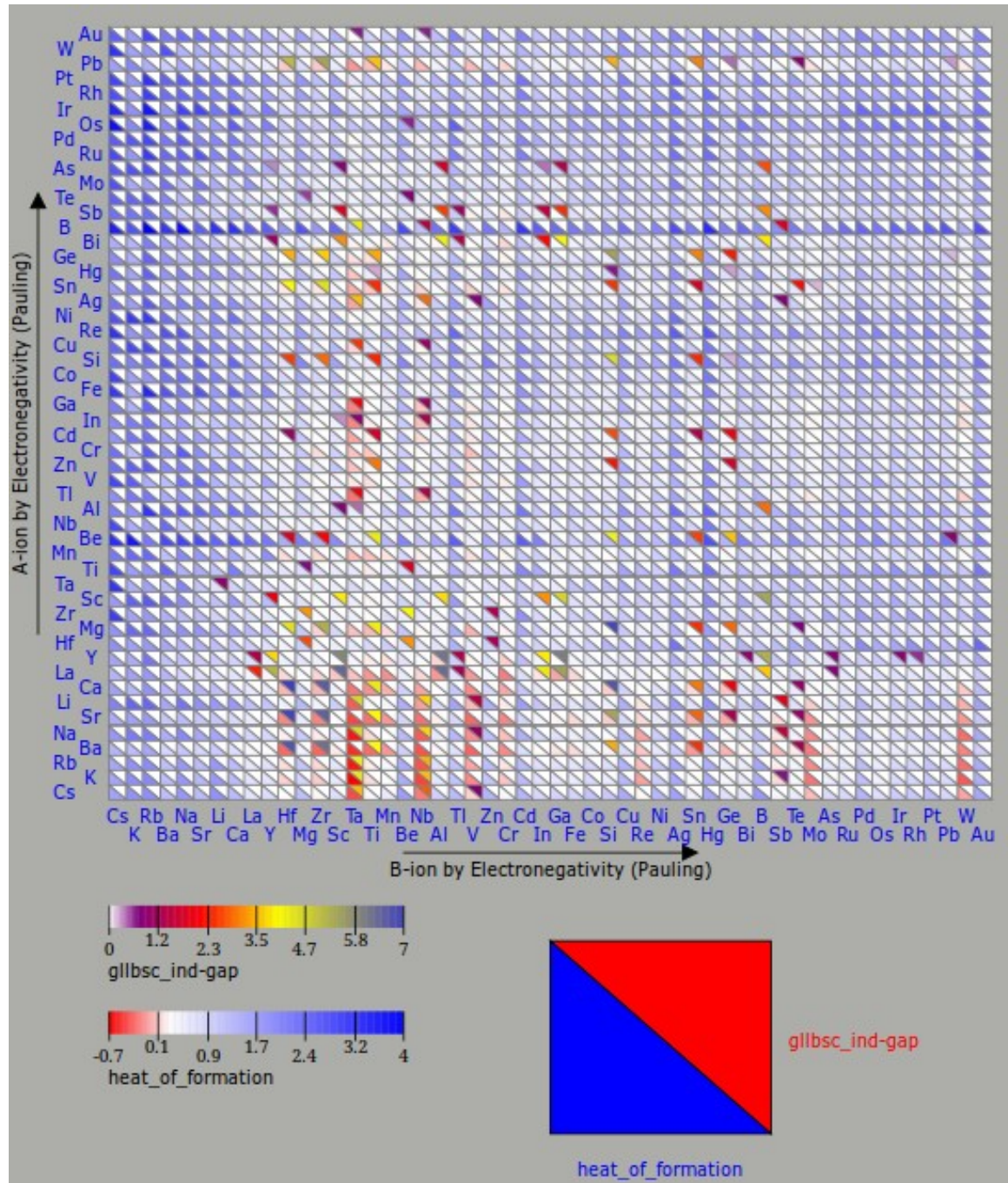
Update matrix

**Update matrix:**

I am done with the settings, show me the resulting heat map!

# Heat Map

Heat map resulting from the default values in the search box as in [1].

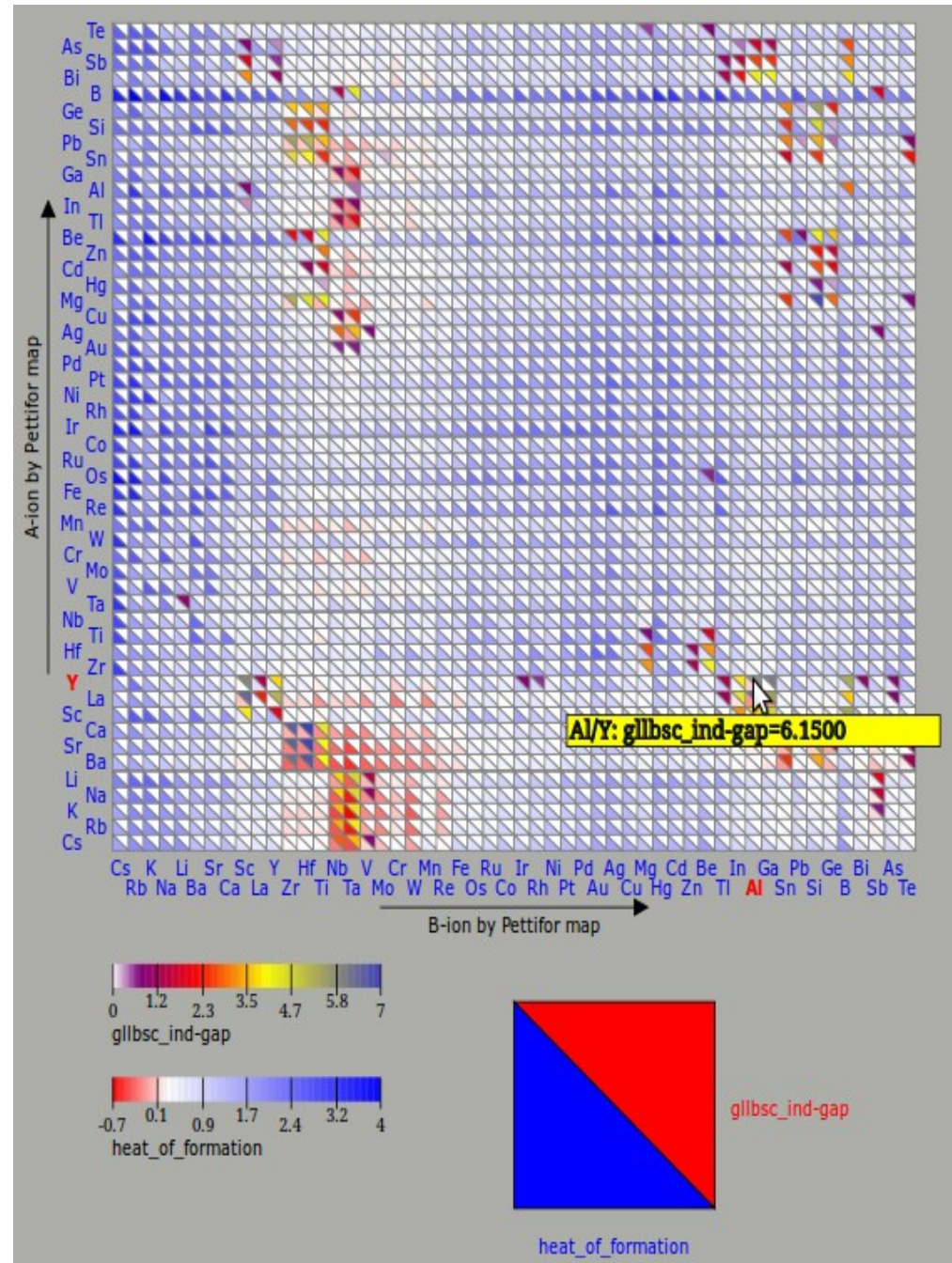




Heat map using the Pettifor map as order.

Information about the composition and value of each triangle comes out with a mouse movement on the heat map.

A click on each combination-square opens the band edges analysis or the calculation data.



Search box

## Computational Materials Repository

Data table

[Hide search box](#)[go to the heatmap interface](#)

Combination: ABO3

Keywords:

Restriction 1:

Restriction 2:

Restriction 3:

Restriction 4:

Update

Restrict the result to contain ALL selected atoms:  
(If none are chosen all atoms are allowed.)

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
Fr	Ra	Ac**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Uuq	Uup	Uuh	Uus	Uuo
	*	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
	**	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Update

« 1 2 3 4 5 6 7 8 9 ... 271 »

id_ref	A	B	anion	heat_of_formation	gllbsc_dir-gap	gllbsc_ind-gap	atoms	db_keywords	db_description	doi	download
<a href="#">4</a>	Sn	Si	O3	0.53	4.27	2.54	O Si Sn (30, 1Si, 1Sn)	ABO3 max O O3 perovskite Si Sn SnSiO3	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	
<a href="#">10</a>	Os	Sb	O3	1.55	0	0	O Os Sb (30, 10s, 1Sb)	ABO3 max O O3 perovskite Os OsSbO3 perovskite Sb	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	
<a href="#">11</a>	Mo	Ni	O3	1.31	0	0	Mo Ni O (1Mo, 1Ni, 3O)	ABO3 Mo MoNiO3 max Ni O O3 perovskite	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	
<a href="#">15</a>	Co	As	O3	1.01	0	0	As Co O (1As, 1Co, 3O)	ABO3 As Co CoAsO3 max O O3 perovskite	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	
<a href="#">16</a>	Mo	Ga	O3	0.70	0	0	Ga Mo O (1Ga, 1Mo, 3O)	ABO3 Ga Mo MoGaO3 max O O3 perovskite	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	
<a href="#">21</a>	B	Mn	O3	1.52	0	0	B Mn O (1B, 1Mn, 3O)	ABO3 B BMnO3 Mn max O O3 perovskite	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	
<a href="#">23</a>	Ti	Hg	O3	2.35	0	0	Hg O Ti (1Hg, 3O, 1Ti)	ABO3 Hg max O O3 perovskite Ti TiHgO3	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	
<a href="#">24</a>	Cd	K	O3	2.32	0	0	Cd K O (1Cd, 1K, 3O)	ABO3 Cd CdKO3 K max O O3 perovskite	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	
<a href="#">26</a>	W	Rh	O3	1.56	0	0	O Rh W (3O, 1Rh, 1W)	ABO3 max O O3 perovskite Rh W WRhO3	Screening cubic perovskite structures, metal oxides	<a href="#">10.1039/b000000x</a>	

[Hide search box](#)

>[go to the heatmap interface](#)<

Combination:

Keywords:

Restriction 1:  <

Restriction 2:  <

Restriction 3:  <

Restriction 4:  <

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

Restrict the result to contain ALL selected atoms:  
(If none are chosen all atoms are allowed.)

H																He	
<input type="checkbox"/>																<input type="checkbox"/>	
Li	Be										B	C	N	O	F	Ne	
<input type="checkbox"/>	<input type="checkbox"/>										<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	
Na	Mg										Al	Si	P	S	Cl	Ar	
<input type="checkbox"/>	<input type="checkbox"/>										<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Fr	Ra	Ac**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Uuq	Uup	Uuh	Uus	Uuo
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	*	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
	**	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		
		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		

Here the user can restrict his search to some criteria, such as stability or size of the gap, and see in the data table which combinations fulfill the requirements.

**Combination and References:**

As in the heat map



[Hide search box](#)

>[go to the heatmap interface](#)<

Combination: ABO3

Keywords:

Restriction 1:

Restriction 2:

Restriction 3:

Restriction 4:

Update

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

Restrict the result to contain ALL selected atoms:  
(If none are chosen all atoms are allowed.)

H <div></div>																He <div></div>	
Li <div></div>	Be <div></div>											B <div></div>	C <div></div>	N <div></div>	O <div></div>	F <div></div>	Ne <div></div>
Na <div></div>	Mg <div></div>											Al <div></div>	Si <div></div>	P <div></div>	S <div></div>	Cl <div></div>	Ar <div></div>
K <div></div>	Ca <div></div>	Sc <div></div>	Ti <div></div>	V <div></div>	Cr <div></div>	Mn <div></div>	Fe <div></div>	Co <div></div>	Ni <div></div>	Cu <div></div>	Zn <div></div>	Ga <div></div>	Ge <div></div>	As <div></div>	Se <div></div>	Br <div></div>	Kr <div></div>
Rb <div></div>	Sr <div></div>	Y <div></div>	Zr <div></div>	Nb <div></div>	Mo <div></div>	Tc <div></div>	Ru <div></div>	Rh <div></div>	Pd <div></div>	Ag <div></div>	Cd <div></div>	In <div></div>	Sn <div></div>	Sb <div></div>	Te <div></div>	I <div></div>	Xe <div></div>
Cs <div></div>	Ba <div></div>	La* <div></div>	Hf <div></div>	Ta <div></div>	W <div></div>	Re <div></div>	Os <div></div>	Ir <div></div>	Pt <div></div>	Au <div></div>	Hg <div></div>	Tl <div></div>	Pb <div></div>	Bi <div></div>	Po <div></div>	At <div></div>	Rn <div></div>
Fr <div></div>	Ra <div></div>	Ac** <div></div>	Rf <div></div>	Db <div></div>	Sg <div></div>	Bh <div></div>	Hs <div></div>	Mt <div></div>	Ds <div></div>	Rg <div></div>	Cn <div></div>	Uut <div></div>	Uuq <div></div>	Uup <div></div>	Uuh <div></div>	Uus <div></div>	Uuo <div></div>
	*	Ce <div></div>	Pr <div></div>	Nd <div></div>	Pm <div></div>	Sm <div></div>	Eu <div></div>	Gd <div></div>	Tb <div></div>	Dy <div></div>	Ho <div></div>	Er <div></div>	Tm <div></div>	Yb <div></div>	Lu <div></div>		
	**	Th <div></div>	Pa <div></div>	U <div></div>	Np <div></div>	Pu <div></div>	Am <div></div>	Cm <div></div>	Bk <div></div>	Cf <div></div>	Es <div></div>	Fm <div></div>	Md <div></div>	No <div></div>	Lr <div></div>		

Update

## Keywords:


Identifier for a group of calculations. It can be the chemical formula, the anion composition...

[Hide search box](#)

>[go to the heatmap interface](#)<

Combination: ABO3

Keywords:

Restriction 1:  < <

Restriction 2: < <

Restriction 3: < <

Restriction 4: < <

Update

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

Restrict the result to contain ALL selected atoms:  
(If none are chosen all atoms are allowed.)

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
Fr	Ra	Ac**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Uuq	Uup	Uuh	Uus	Uuo
	*	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
	**	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Update

## Restriction #:

Requirements that the data must fulfill.

Restriction available:

- heat of formation;
- size of the gap.

(in a not-to-far-future also band edges position).

[Hide search box](#)

>[go to the heatmap interface](#)<

Combination: ABO3

Keywords:

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

Restriction 1:

Restriction 2:

Restriction 3:

Restriction 4:

Update

Restrict the result to contain ALL selected atoms:  
(If none are chosen all atoms are allowed.)

H <div></div>																He <div></div>	
Li <div></div>	Be <div></div>											B <div></div>	C <div></div>	N <div></div>	O <div></div>	F <div></div>	Ne <div></div>
Na <div></div>	Mg <div></div>											Al <div></div>	Si <div></div>	P <div></div>	S <div></div>	Cl <div></div>	Ar <div></div>
K <div></div>	Ca <div></div>	Sc <div></div>	Ti <div></div>	V <div></div>	Cr <div></div>	Mn <div></div>	Fe <div></div>	Co <div></div>	Ni <div></div>	Cu <div></div>	Zn <div></div>	Ga <div></div>	Ge <div></div>	As <div></div>	Se <div></div>	Br <div></div>	Kr <div></div>
Rb <div></div>	Sr <div></div>	Y <div></div>	Zr <div></div>	Nb <div></div>	Mo <div></div>	Tc <div></div>	Ru <div></div>	Rh <div></div>	Pd <div></div>	Ag <div></div>	Cd <div></div>	In <div></div>	Sn <div></div>	Sb <div></div>	Te <div></div>	I <div></div>	Xe <div></div>
Cs <div></div>	Ba <div></div>	La* <div></div>	Hf <div></div>	Ta <div></div>	W <div></div>	Re <div></div>	Os <div></div>	Ir <div></div>	Pt <div></div>	Au <div></div>	Hg <div></div>	Tl <div></div>	Pb <div></div>	Bi <div></div>	Po <div></div>	At <div></div>	Rn <div></div>
Fr <div></div>	Ra <div></div>	Ac** <div></div>	Rf <div></div>	Db <div></div>	Sg <div></div>	Bh <div></div>	Hs <div></div>	Mt <div></div>	Ds <div></div>	Rg <div></div>	Cn <div></div>	Uut <div></div>	Uuq <div></div>	Uup <div></div>	Uuh <div></div>	Uus <div></div>	Uuo <div></div>
	*	Ce <div></div>	Pr <div></div>	Nd <div></div>	Pm <div></div>	Sm <div></div>	Eu <div></div>	Gd <div></div>	Tb <div></div>	Dy <div></div>	Ho <div></div>	Er <div></div>	Tm <div></div>	Yb <div></div>	Lu <div></div>		
	**	Th <div></div>	Pa <div></div>	U <div></div>	Np <div></div>	Pu <div></div>	Am <div></div>	Cm <div></div>	Bk <div></div>	Cf <div></div>	Es <div></div>	Fm <div></div>	Md <div></div>	No <div></div>	Lr <div></div>		

Update

Update!!

Update

**Selection of atoms:**  
Restrict the search on a particular set of atoms  
(All if none are chosen).

Water splitting candidates in ABO<sub>2</sub>N composition:> [go to the heatmap interface](#) <Combination: ABO<sub>2</sub>N

Keywords:

Restriction 1: heat\_of\_formation (eV) &lt; 0.2

Restriction 2: glbbsc\_ind-gap (eV) &lt; 3

Restriction 3: glbbsc\_ind-gap (eV) &gt; 1.5

Restriction 4: &lt;

Update

Restrict the result to contain ALL selected atoms:  
(If none are chosen all atoms are allowed.)

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 ☐
Fr ☐	Ra ☐	Ac** ☐	Rf ☐	Db ☐	Sg ☐	Bh ☐	Hs ☐	Mt ☐	Ds ☐	Rg ☐	Cn ☐	Uut ☐	Uuq ☐	Uup ☐	Uuh ☐	Uus ☐	Uuo ☐
	*	Ce ☐	Pr ☐	Nd ☐	Pm ☐	Sm ☐	Eu ☐	Gd ☐	Tb ☐	Dy ☐	Ho ☐	Er ☐	Tm ☐	Yb ☐	Lu ☐		
	**	Th ☐	Pa ☐	U ☐	Np ☐	Pu ☐	Am ☐	Cm ☐	Bk ☐	Cf ☐	Es ☐	Fm ☐	Md ☐	No ☐	Lr ☐		



















Update

References:

- ☒ abn
- ☒ abox
- ☒ an
- ☒ aox
- ☒ aoxn
- ☒ bulk

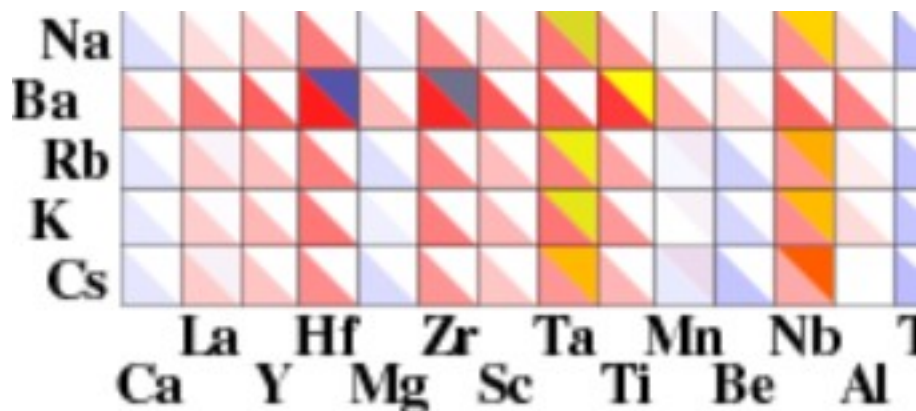
id_ref	A	B	anion	heat_of_formation	glbbsc_dir-gap	glbbsc_ind-gap	atoms	db_keywords	db_description	doi	downloads
<a href="#">174</a>	Ca	Ta	O2N	0.03	2.22	2.22	N O Ca Ta (1N, 2O, 1Ca, 1Ta)	ABO <sub>2</sub> N Ca CaTaNO <sub>2</sub> moxn N O O2N perovskite Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="#">10.1039/b000000x</a>	
<a href="#">473</a>	Sr	Ta	O2N	-0.12	2.15	2.15	N O Sr Ta (1N, 2O, 1Sr, 1Ta)	ABO <sub>2</sub> N moxn N O O2N perovskite Sr SrTaNO <sub>2</sub> Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="#">10.1039/b000000x</a>	
<a href="#">981</a>	Pb	Ta	O2N	0.13	2.07	1.95	N O Ta Pb (1N, 2O, 1Ta, 1Pb)	ABO <sub>2</sub> N moxn N O O2N Pb PbTaNO <sub>2</sub> perovskite Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="#">10.1039/b000000x</a>	
<a href="#">1929</a>	La	Ti	O2N	0.05	2.49	2.49	N O Ti La (1N, 2O, 1Ti, 1La)	ABO <sub>2</sub> N La LaTiNO <sub>2</sub> moxn N O O2N perovskite Ti	Screening cubic perovskite structures, metal oxynitrides	<a href="#">10.1039/b000000x</a>	
<a href="#">3884</a>	Ba	Ta	O2N	-0.18	2.05	2.05	N O Ba Ta (1N, 2O, 1Ba, 1Ta)	ABO <sub>2</sub> N Ba BaTaNO <sub>2</sub> moxn N O O2N perovskite Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="#">10.1039/b000000x</a>	
<a href="#">4989</a>	Mg	Nb	O2N	0.18	2.03	1.51	N O Mg Nb (1N, 2O, 1Mg, 1Nb)	ABO <sub>2</sub> N Mg MgNbNO <sub>2</sub> moxn N Nb O O2N perovskite	Screening cubic perovskite structures, metal oxynitrides	<a href="#">10.1039/b000000x</a>	
<a href="#">5344</a>	Mg	Ta	O2N	0.13	2.73	2.08	N O Mg Ta (1N, 2O, 1Mg, 1Ta)	ABO <sub>2</sub> N Mg MgTaNO <sub>2</sub> moxn N O O2N perovskite Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="#">10.1039/b000000x</a>	

## Water splitting candidates in ABO<sub>2</sub>N composition:

id_ref	A	B	anion	heat_of_formation	glibsc_dir-gap	glibsc_ind-gap	atoms	db_keywords	db_description	doi	downloads
<a href="#">174</a>	Ca	Ta	O2N	0.03	2.22	2.22	N O Ca Ta (1N, 2O, 1Ca, 1Ta)	ABO2N Ca CaTaNO2 moxn N O O2N perovskite Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="https://doi.org/10.1039/b000000x">10.1039/b000000x</a>	  
<a href="#">473</a>	Sr	Ta	O2N	-0.12	2.15	2.15	N O Sr Ta (1N, 2O, 1Sr, 1Ta)	ABO2N moxn N O O2N perovskite Sr SrTaNO2 Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="https://doi.org/10.1039/b000000x">10.1039/b000000x</a>	  
<a href="#">981</a>	Pb	Ta	O2N	0.13	2.07	1.95	N O Ta Pb (1N, 2O, 1Ta, 1Pb)	ABO2N moxn N O O2N Pb PbTaNO2 perovskite Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="https://doi.org/10.1039/b000000x">10.1039/b000000x</a>	  
<a href="#">1929</a>	La	Ti	O2N	0.05	2.49	2.49	N O Ti La (1N, 2O, 1Ti, 1La)	ABO2N La LaTiNO2 moxn N O O2N perovskite Ti	Screening cubic perovskite structures, metal oxynitrides	<a href="https://doi.org/10.1039/b000000x">10.1039/b000000x</a>	  
<a href="#">3884</a>	Ba	Ta	O2N	-0.18	2.05	2.05	N O Ba Ta (1N, 2O, 1Ba, 1Ta)	ABO2N Ba BaTaNO2 moxn N O O2N perovskite Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="https://doi.org/10.1039/b000000x">10.1039/b000000x</a>	  
<a href="#">4989</a>	Mg	Nb	O2N	0.18	2.03	1.51	N O Mg Nb (1N, 2O, 1Mg, 1Nb)	ABO2N Mg MgNbNO2 moxn N Nb O O2N perovskite	Screening cubic perovskite structures, metal oxynitrides	<a href="https://doi.org/10.1039/b000000x">10.1039/b000000x</a>	  
<a href="#">5344</a>	Mg	Ta	O2N	0.13	2.73	2.08	N O Mg Ta (1N, 2O, 1Mg, 1Ta)	ABO2N Mg MgTaNO2 moxn N O O2N perovskite Ta	Screening cubic perovskite structures, metal oxynitrides	<a href="https://doi.org/10.1039/b000000x">10.1039/b000000x</a>	  

(in order of appearance):  
 Id of the calculation;  
 A- and B-ion;  
 Heat of formation;  
 Direct bandgap;  
 Indirect bandgap;  
 Atomic composition;  
 Keywords,  
 Data description;  
 DOI of the paper  
 relative to the data;  
 Download the data in  
 different formats.





Please, remember to cite:

[1] I.E. Castelli, T. Olsen, S. Datta, D.D. Landis, K.S. Thygesen, S. Dahl, K.W. Jacobsen, Energy & Environmental Science, in printing.

[2] Computational Materials Repository, <https://cmr.fysik.dtu.dk/>.

[3] The papers corresponding to the data you have used (the DOI is in the data table).

Thanks!

Data provided and mantained by Ivano E. Castelli

Database devellopped by David Landis

For questions about the data, please contact [ivano.castelli\(at\)fysik.dtu.dk](mailto:ivano.castelli@fysik.dtu.dk)