Quick reference of the interactive structure map of AB_2 type 2D materials by high-throughput DFT calculations

The website provides an interactive structure map of AB_2 type 2D materials constructed by high-throughput DFT calculations. All the details of the maps can be found in arXiv: 1904.06047 [cond-mat.mtrl-sci].

http://www.openmx-square.org/2d-ab2/

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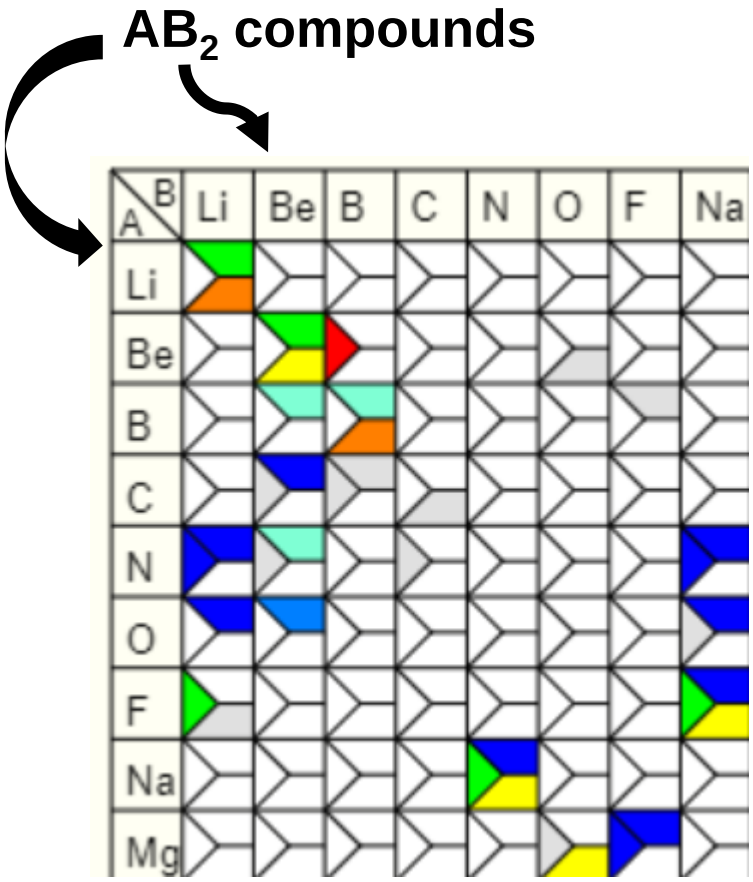
Legend



- In the table the column and row represent species A and B in AB_2 compounds, while they can be reversed by checking as

Reverse A ⇔ B ☑

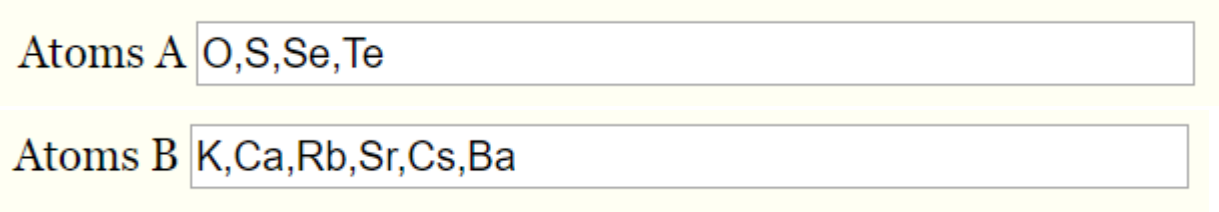
- Each block has three segments corresponding to its initial structure for the optimization, where ‘P’, ‘T’, and ‘H’ mean a planar, 1T, and 1H structure.

- The color stands for the final structure specified by the space group determined with a tolerance or characteristic features.

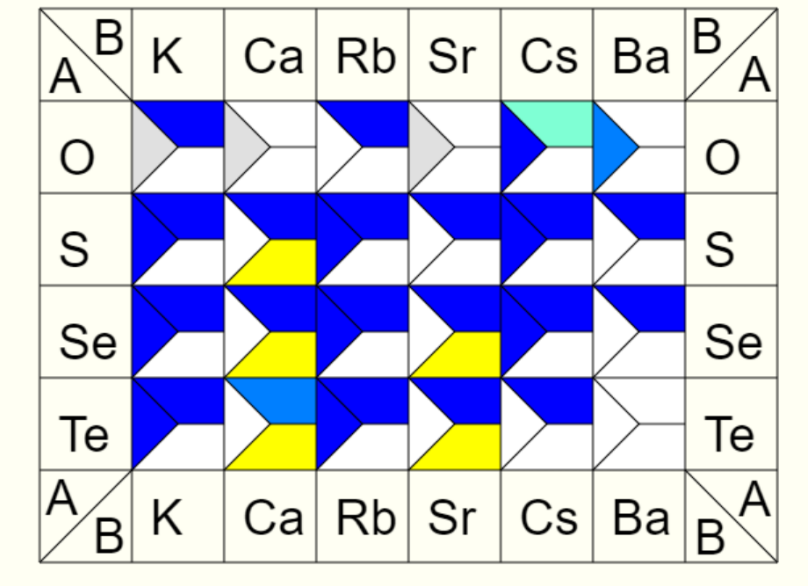
where the white color corresponds to compounds which did not converge or converged to a structure with a relative energy more than 0.82 eV/(12 atoms) compared to the most stable structure.

Choice of species

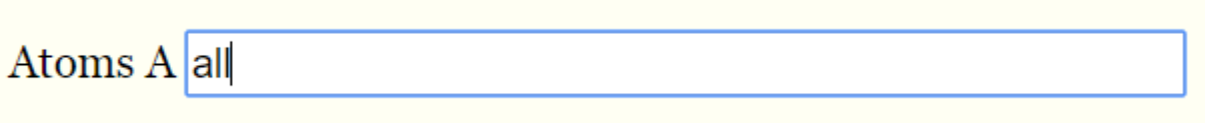
- The structure map will be restructured by specifying atomic symbols separated by a comma in forms of 'Atoms A' and 'Atoms B‘.



- Then, you will see the following structure map on your browser.

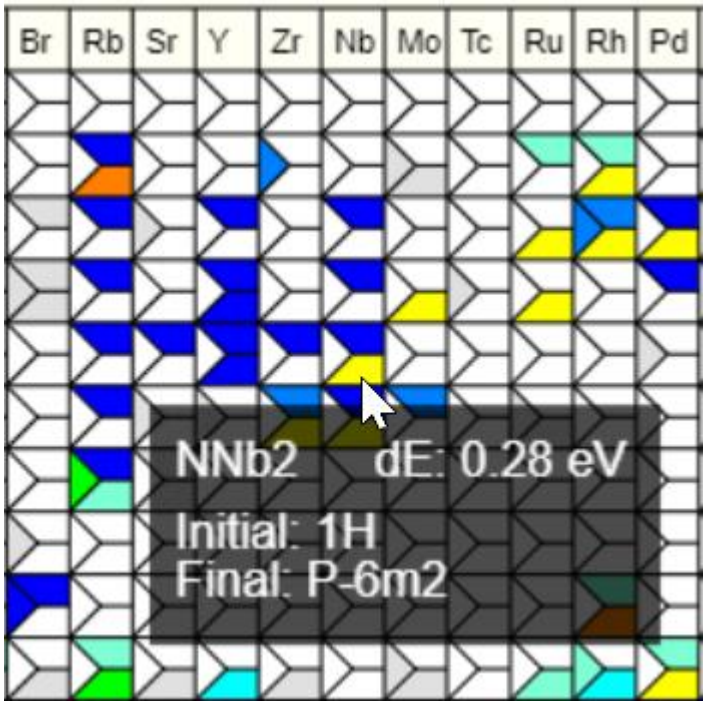


- By typing ‘all’, all the 62 elements we considered will be selected.



Hover information

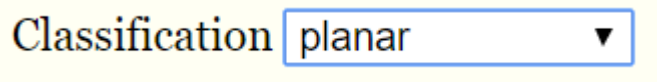
- Information of a segment arrowed by the mouse pointer will appear as shown below.



- The hover box contains the name of compound, the initial and final structures, and the relative energy in eV with respect to the lowest energy among convergent structures in three segments. The relative energy of structures corresponding to the white box is not shown.

List of compounds

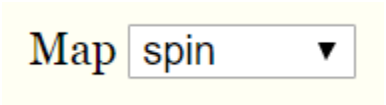
- It is possible to list all 2D compounds specified by either a space group or a characteristic structure in a form of 'Classification'.



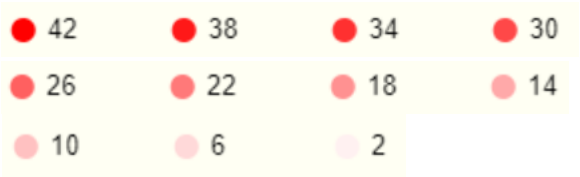
- Then, you will see the following list:

Spin map

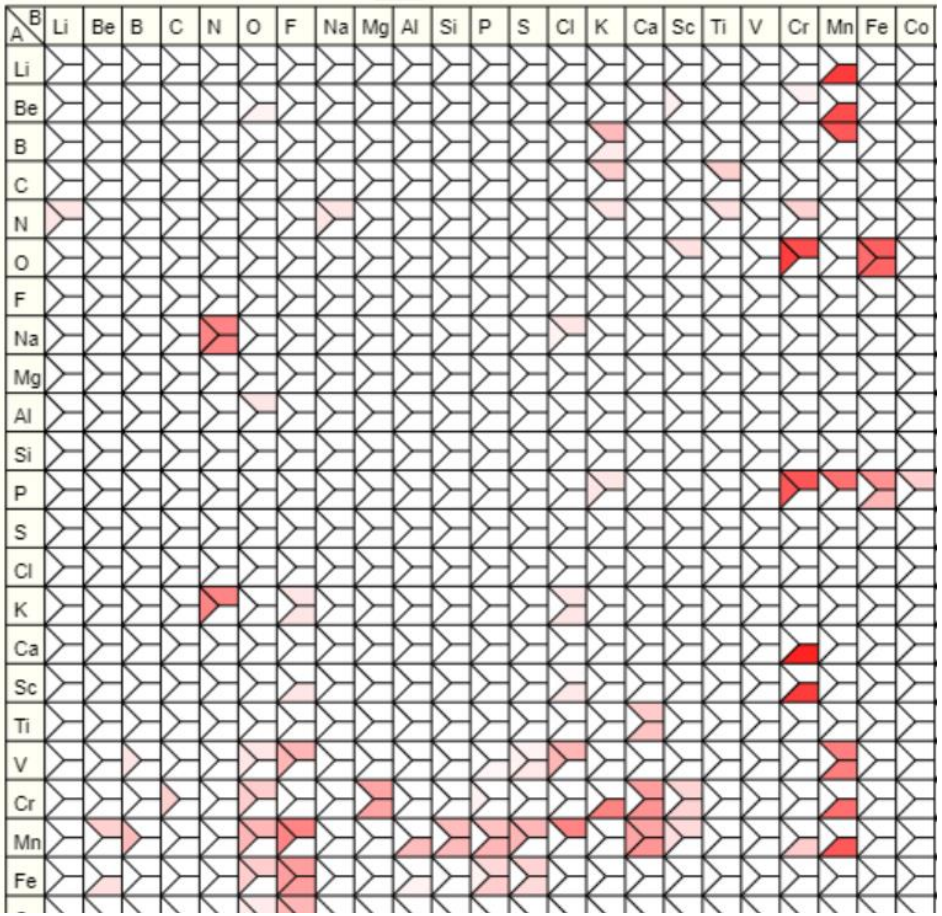
- In addition to the structure map, one can see a spin map by specifying 'spin' in a form of 'Map', where compounds with larger total magnetic moments per 12 atoms are colored by a vivid red.



- Then, you will see the following spin map:
- The color corresponds to the total magnetic moment (μ_B) per 12 atoms.

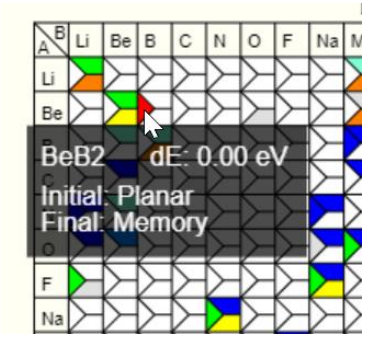


- It should be noted that the magnetic state may not be the ground state one, since we started the ferromagnetic state in all the optimizations.



Viewer

- By clicking a colored region, you can jump a page containing detailed information.
- The following new window will pop up.



- In the window you can confirm how the structure changed during the optimization, while a part of optimization steps are shown for some of structures due to many trials of optimization. The optimized lattice parameters in angstrom and degree, total energy in Hartree, and the total magnetic moment in μ_B are shown in the right top.
- The cif and md files can be downloaded.
- In the near future, we are going to add DOS and band structure in the page.