**Extraction of data from .bxsf files**

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3. **Using the code operation**

The present code extracts the (3D) bandstructure data in a .bxsf format file and makes a file in the form required by the EMAF code. The folder contains the following files:

* Main\_Data\_Extraction, this is the code that needs to be modified in its early lines (16 to 32) and launched. It opens the other scripts as required.
* Data\_from\_bxsf reads the data from the bxsf file
* BandMatrix\_to\_Ek\_v2 composes the Ek matrix file and the ***k*** axes coordinates matrixes, allowing different size of the *k*-mesh in the three space directions.

Please, be aware that the code assumes the units of the energy to be eV and does not modify them.

1. **Writing the instructions**

The instructions are contained in the lines 16 to 32 of the Main file. Below we report and explain these lines, using as example the case of Mg3Sb2.

% input information

fileName = 'Mg3Sb2\_fs.bxsf'; % name of the bxsf file

material\_name = 'Mg3Sb2\_trial; % material name that will be used to save the band structure as Ek\_'material\_name'

num\_of\_bands = 5; % write the number of bands in the file

points\_in\_axis\_kx = 61; % write the number of points in the k space

points\_in\_axis\_ky = 61;

points\_in\_axis\_kz = 41;

num\_elements\_each\_row = 6; % how many energy values in each row

Fermi = 7.2709; % in eV, value of the Fermi level.

% In the Ek file, it will be placed to zero, NOTE!

alat = 0.4597;

fileName is the name of the .bxsf file from which we want to extract the data.

material\_name is the name that will be used to save the extracted data in the form Ek\_’material\_name’.

num\_of\_bands is the number of bands, or of eigenvalues, and is usually in the line 13 of the .bxsf file

points\_in\_axis\_kx/y/z is the number of points in each axis of the *k-*mesh, is usually contained in the line 14 of the .bxsf file.

num\_elements\_each\_row is the number of energy values that are in each row.

Fermi is the Fermi level position in eV. It is usually in the line 8 of the bxsf file and will be set to zero for the EMAF code usage.

alat is the lattice constant, in nm. Please, note that the alat value is not usually contained in the .bxsf file but should be known. It is important as the reciprocal unit cell vectors are in units of 2*p*/alat