Tutorial: Computing the Magnetic Anisotropy Surface for Fe^{3+} embedded in a $PbTiO_3$ host

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: https://github.com/nimalec/Magmango

In this tutorial, we use Magmango package to compute the three-dimensional magnetocrystalline anisotropy (MCAE) surface of a Fe3+ ion embedded in the $PbTiO_3$ ferroelectric host. The requirements for the setup can be found in the requirements.txt file of the Magmango repository. First, run the following command on the command line to set up Magmango.

```
git clone git@github.com:nimalec/Magmango.git
```

Once this step is complete, run the following.

```
python setup.py
```

If no errors are present, you have successfully set up the working environment. The next step will be to obtain a relaxed structure of the system of interest and insure that the parameters used in the structural relaxation are consistent with those in . For this example, we will consider Fe^3 substituting a Ti site in a $PbTiO_3$ supercell comprising 135 atoms. Hence, we will use the corresponding VASP POSCAR file for our MCAE predictions. Our implementation will involve two steps (1) a single spin collinear total energy calculation and (2) a set of spin non-collinear calculations. We will implement the collinear step. Create a python file clexecute.py with the following

```
from magmango.calculation.calculation import Calculation
from magmango.calculation import kpoints.KPointsSettings as KPoints, poscar.PoscarSettings as
    Poscar, potcar.PotcarSettings as Potcar, incar.IncarSettings as Incar,
    runscript.RunscriptSettings as Runscript

dir_cl = "directory/collinear"
incar_path = "directory/INCAR"
poscar_path = "directory/POSCAR"
potcar_path = "directory/POTCAR"
kpoints_path = "directory/KPOINTS"
runscript_path = "directory/runscript.sh"
incar_obj = Incar(from_file = True)
kpoints_obj = KPoints(from_file = True)
poscar_obj = Poscar(from_file = True )
potcar_obj = Potcar(from_file = True)
runscript_obj = Runscript(from_file = True)
incar_obj.incar_from_file(incar_path)
kpoints_obj.incar_from_file(kpoints_path)
poscar_obj.incar_from_file(poscar_path)
potcar_obj.incar_from_file(potcar_path)

calculation = Calculation(dir_cl , incar_obj , kpoints_obj, poscar_obj, potcar_obj, runscript_obj )
```

```
calculation.make_calculation()
calculation.run_calculation()
```

Execute the above using,

```
python clexecute.py
```

and wait until the calculation is complete. Next, we perform the spin non-collinear calculations. We will perform this over a grid of 200 points. Do this by creating a file nclexecute.py:

```
from magmango.mae.mae_calc import MagneticAnisotropyFlow
dir_cl = "directory/collinear"
npoints = 200
workdir = "directory/mcae"
mcae = MagneticAnisotropyFlow(workdir = workdir , npoints, cl_dir = dir_cl)
mcae.make_calculations()
mcae.run_ncl_calculations()
```

Then run,

```
python nclexecute.py
```

The above block of code will execute the spin non-collinear calculations. The final step is to extract the list of MCAE points from this series of calculations. For this, execute the following in Python.

```
from magmango.in_out.mae_extraction import mae_outfile_write
workdir = "directory/mcae"
mae_outfile_write(workdir)
```

This should now output a file "mae_output.txt" in "directory/mcae" . This should contain 6 columns: (1) index of the spin, (2) S_x, (3) S_y, (4) S_z, (5) E_{tot}, (6) ΔE_{MCAE}. You did it! You now can use our plotting module (in construction) to generate plots of surfaces and our analysis toolbox (in construction) to extract the MCAE tensor elements.