Set_up_Runs_Example

November 23, 2018

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In [1]: # Set up a relaxation run using the VASP input file templates
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In [87]: # Import the mods
         import pymatgen as mg
         from pymatgen.io.vasp.inputs import *
         import os, shutil, glob
```

```
In [88]: # our cwd:
         # Contains a template INCAR and KPOINTS, a POTCAR for Mo and S and the two POSCAR files
         os.listdir()
```

```
Out[88]: ['POSCAR_MoS2_Bulk',
          'POSCAR_MoS2_2D',
          '.ipynb_checkpoints',
          'INCAR.relax',
          'job.submit.file',
          'mo2.s4',
          'Untitled.ipynb',
          'KPOINTS.relax',
          'POTCAR_Mo_S']
```

```
In [89]: # make a list of poscars to loop through...
         poslist = glob.glob('POSCAR*')
         poslist
```

```
Out[89]: ['POSCAR_MoS2_Bulk', 'POSCAR_MoS2_2D']
```

```
In [95]: # make a loop to set up relax run directories:
         for pos in poslist:
             # import a pymatgen structure object
             cell = mg.Structure.from_file(pos)

             # create a unique id for run sub directory
             fid = '.'.join(cell.formula.split()).lower()

             # get INCAR,KPOINTS,and POTCAR
             incar = Incar.from_file('INCAR.relax')
             kpoints = Kpoints.from_file('KPOINTS.relax')
```

```python
potcar = Potcar.from_file('POTCAR_Mo_S')

# special case for 2D
if '2D' in pos:
    kpoints.kpts[0][2] = 1
else:
    pass

# Add VASP objects and generate subdirectories
vaspin = VaspInput(incar=incar,
        kpoints=kpoints,
        poscar=pos,
        potcar=potcar)

vaspin.write_input(output_dir=fid,
                make_dir_if_not_present=True)

# Copy the job submit file to the run subdirectories
os.system('cp job.submit.file {}/'.format(fid))
```

In [ ]:

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