Running the OLED DFT Workflow

This is a minimal guide to running my DFT workflow. The first step is to install Pylada (see the Installation section of the other tutorial).

Setting up the calculations

Making the input files

The first thing you will need is a folder containing all the molecules in the POSCAR form. I convert the files using Open Babel. but the resulting POSCARS have 0 unit cells so I use a different script to add a unit cell to the files. If you have obabel and Pylada installed, you can use the script *tovasp.sh* to do this automatically:

```
bash tovasp.sh dir_containing_mols/
```

This will create a folder named `POSCARs` with the converted POSCARs. You need to make sure the file `center.py` is in the current directory.

> **Note**
>
> If you want the scripts to work out of the box, the POSCARs need to be named in the form `POSCAR_[entry]`.

Run directory

On the supercomputer create a directory in `scratch` with the following files and folders:

```
POSCARs #the directory we just created
mols #a directory containing the equivalent entries in mol format
interp.py
reposition.py
stretch.py
extract_images.py
extract_data.py
mcu.py
HT_workflow.ipy
```

Open `HT_workflow.ipy`, at lines 29-30 set the location of the VASP executable and the pseudo-potentials:

```
############### setting up the functional
vasp=Relax()
vasp.has_nlep = False

vasp.program = '/scinet/niagara/software/commercial/vasp-6.1.2/bin/vasp_ncl' #<- this line
pseudoDir = '/scinet/niagara/software/commercial/vasp-6.1.2/potpaw_PBE/' #<- and this line

vasp.add_specie = "C", pseudoDir + "/C"
vasp.add_specie = "H", pseudoDir + "/H"
```

> Note
>
> You need to specify the path to `vasp_ncl` because spin orbit coupling requires non-collinear calculations.

Then, in your `home` directory create a directory named `pylada_chains` and add `OLED_workflow_dryrun.py` to it. Then add the following to your `~/.bashrc`:

```
export PYTHONPATH=:$PYTHONPATH:$HOME/pylada_chains
export VASP_PP_PATH="/scinet/niagara/software/commercial/vasp-6.1.2/" # <-- Path to vasp for ASE
```

The second line contains the path to VASP for ASE to read. Don't forget to source your `~/.bashrc`:

```
source ~/.bashrc
```

Additional required packages

In the python environment where you have installed Pylada. You will have to install the following python packages:

```
pip install ase pymatgen rdkit
```

Launching the calculations

To launch calculations go to the directory you just created in `scratch` and to this:

```
ipython
In [1]: %run HT_workflow.ipy
In [2]: %launch scattered --account=rrg-ovoznyy --walltime=24:00:00 --ppn=40 --queue=compute
```

You can adjust the launch command according to the computer you are working on and the allocation you want to use. This will launch calculations for all the molecules in the `POSCARs` directory. If calculations hit the wall time, you can safely repeat this step, jobs that are finished will finish as soon as they start and won't be overwritten and jobs that did not finish will continue where they left off.

Extracting the results

Once all calculations are finished, use the following to get a text file containing all the results:

```
python extract_data.py
```

This will create a text file named `results.txt` with the following structure:

file name	Energy Gap	k_r	Iridium Spin Orbit Coupling Energy	Activation barrier (not relaxed)	Activation barrier (relaxed)	weakest bond strength

To obtain wavelength

$\lambda = \frac{1240}{E_{gap}}$

k_r is consistently overestimated, so I adjust it with

$k_r = \frac{k_r}{15}$

k_{nr} is obtained with:

$k_{nr} = k_{nr}(T) + k_{ISC} = Ae^{-\frac{E_{rel}}{Bk_BT}} + Ce^{-E_{gap}} = 10^7 e^{-\frac{E_{rel}}{3 \times 0.02585}} + 10^5 e^{-E_{gap}}$

Good luck!