

Optical Properties Suite Workflow and Resulting Successes and Failures

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March 2, 2022

Outline

1 Input/Output

2 Results

3 Logistics

Inputs

Structure Selection

- 1 mpID, POSCARs, cifs, etc. made into pymatgen structure
- 2 pmg struct is encoded as dictionary and sent to tool
- 3 Dictionaries can be easily checked for identity

Input Declaration

```
{'@module': 'pymatgen.core.structure',
 '@class': 'Structure',
 'charge': None,
 'lattice': {'matrix': [[1.5920500003918698, -2.7575114888687695, 0.0],
 [1.5920500003918698, 2.7575114888687695, 0.0],
 [0.0, 0.0, 5.1551]],
 'a': 3.1841000007837397,
 'b': 3.1841000007837397,
 'c': 5.1551,
 'alpha': 90.0,
 'beta': 90.0,
 'gamma': 120.00000000000001,
 'volume': 45.26276950032406},
 'sites': [{'species': [{'element': 'Zn', 'occu': 1}],
 'abc': [0.6666666666666666, 0.3333333333333333, 0.5],
 'xyz': [1.5920500003918696, -0.9191704962895898, 2.57755],
 'label': 'Zn',
 'properties': {}},
 {'species': [{'element': 'Zn', 'occu': 1}],
 'abc': [0.3333333333333333, 0.6666666666666666, 0.0],
 'xyz': [1.5920500003918696, 0.9191704962895898, 0.0],
 'label': 'Zn',
 'properties': {}},
 {'species': [{'element': 'O', 'occu': 1}],
 'abc': [0.6666666666666666, 0.3333333333333333, 0.8803099999999999],
 'xyz': [1.5920500003918696, -0.9191704962895898, 4.5380860809999999],
 'label': 'O',
 'properties': {}},
 {'species': [{'element': 'O', 'occu': 1}],
 'abc': [0.3333333333333333, 0.6666666666666666, 0.3803099999999999],
 'xyz': [1.5920500003918696, 0.9191704962895898, 1.9605360809999997],
 'label': 'O',
 'properties': {}}}]}
```

Outputs I

structures/chemistries returned for future query

Outputs can be queried by key and filtered by conditional matching on values

- Formula
- mpID
- spacegroup

Electronic properties returned for analysis

☐ scalars

- ☐ bandgap
- ☐ fermi energy
- ☐ charge densities
- ☐ raman/IR cutoff
- ☐ UV cutoff

☐ spectra

- ☒ raman/IR
- ☐ eDoS
- ☐ phonon dispersion
- ☐ SLME (these might be relegated to post processing)
- ☐ PV FOM

Outputs II

Fallbacks

Kat's Troubleshooting I

Detailed breakdown of simulation shortcomings

- Testing workflow for ZnO (mpid = 2133)
- outputs are **extremely** sensitive to input choices
- trying other structures would be useful as well

ecutwfc = 50 Ry, 1 node

KPOINTS	output
3	Y
6	N (smearing is needed)
9	N (walltime reached)
12	N (walltime reached)
15	N (walltime reached)

Kat's Troubleshooting II

ecutwfc = 50 Ry, 4 nodes

KPOINTS	output
3	Y
6	
9	
12	
15	

ecutwfc = 60 Ry, 4 nodes

Is this too high? ~800 eV, but 'recommended'...

KPOINTS	output
3	N (vc-relax fails)
6	N (vc-relax fails)
9	N (vc-relax fails)

Kat's Troubleshooting III

ecutwfc = 40 Ry, 4 nodes

KPOINTS	output
3	Y
6	N (vc-relax fails)
9	N (vc-relax fails)

Runs Storage

dft related issues presentation.

- Currently very limited by storage space in nanoHUB
- Each (successful) simulation takes up 1-2 GB in storage?
- it may be desirable to reimplement the simtool via a pegasus workflow
 - enabling improved job parallelization?
 - enabling more detailed data management?