# Optical Properties Suite Workflow and Resulting Successes and Failures

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# Outline

# Inputs

## Structure Selection

1. mpID, POSCARS, ciffs, 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, 4.538086080999999],
   '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

- ☐ scalers
  - ☐ bandgap
  - ☐ fermi energy
  - ☐ charge densities
  - ☐ raman/IR cutoff
  - ☐ UV cutoff
- ⊟ spectra
  - ☒ raman/IR
  - ☐ eDoS + Band-structure
  - ☐ phonon dispersion
  - ☐ SLME (these might be relegated to post processing)
  - ☐ PV FOM

# Kat's Troubleshooting in ZnO (mpid = 2133) 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 = 40 Ry, 4 nodes

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

## ecutwfc = 40 Ry, 8 nodes

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

# Kat's Troubleshooting in ZnO (mpid = 2133) II

## 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) |

## ecutwfc = 50 Ry, 4 nodes

| KPOINTS | output |
|---|---|
| 3 | Y |
| 6 | N (vc-relax fails) |
| 9 | Y |
| 12 | N (walltime reached) |
| 15 | N (walltime reached) |

# Kat's Troubleshooting in ZnO (mpid = 2133) III

## 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 in SiC (mpid = 1002206) I

## ecutwfc = 40 Ry, 4 nodes

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

# Convergence Plots I

## Convergence for 3 Kpoints

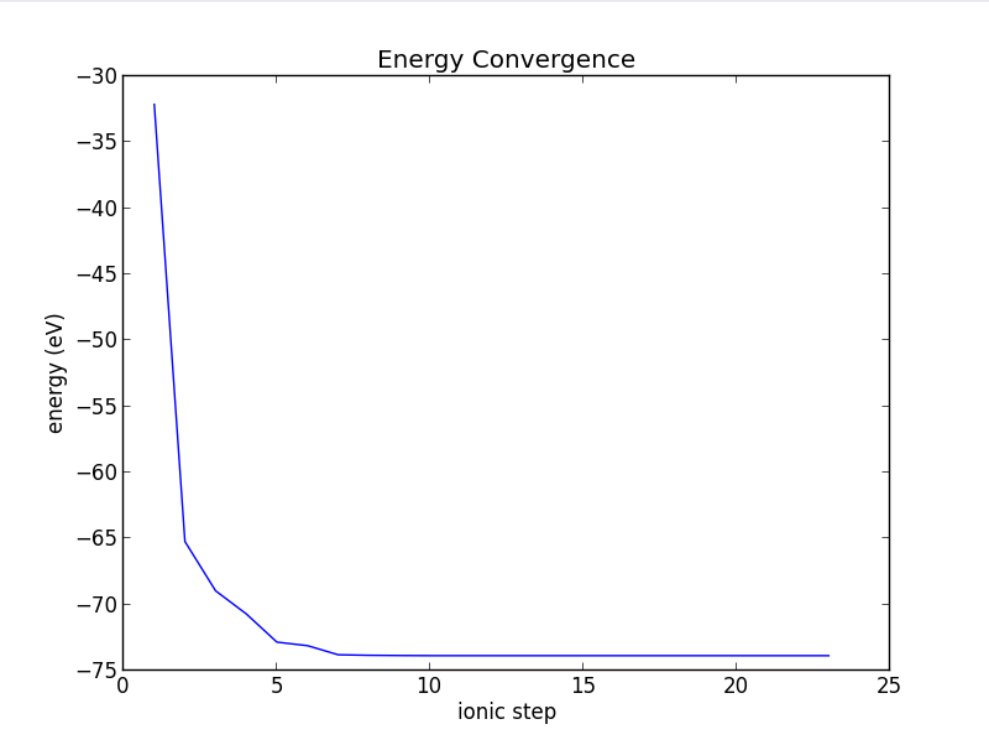


Figure: convergence trend at ecutwfc = 40 Ry

# Convergence Plots II

## 9 Kpoints fails to make any ionic iteration in vcrelax

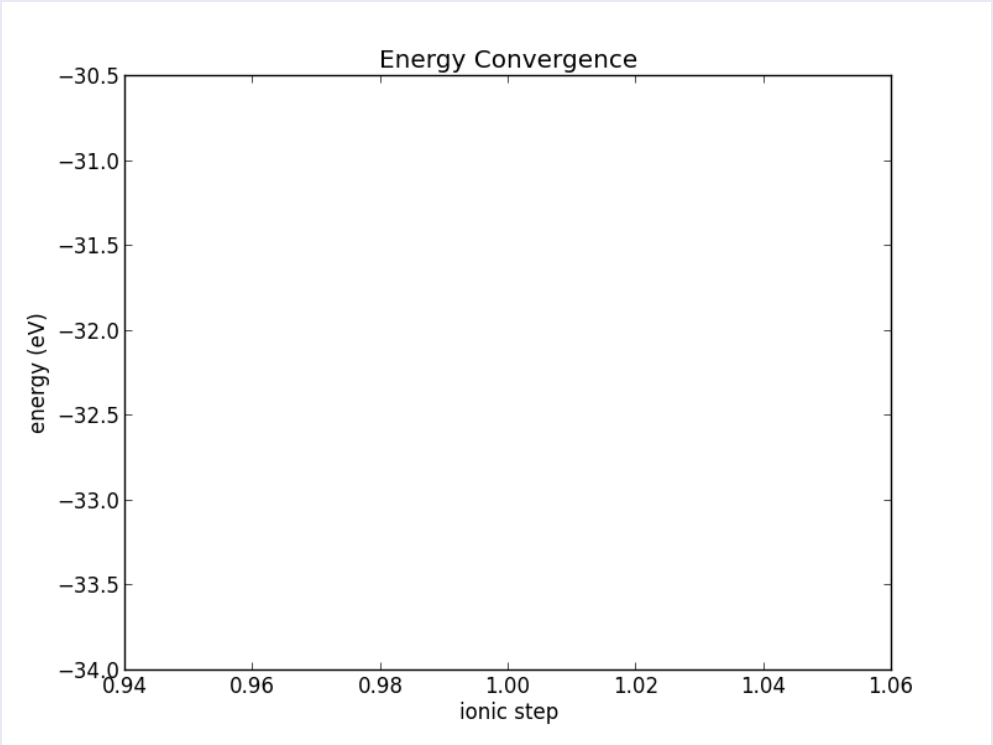


Figure: unfortunately blank at ecutwfc = 40 Ry

# Discussion

- each (successful) simulation takes up 1-2 GB in storage?
- why are they failing to converge?
  - vcrelax final scf calculation fails to converge, even after 1000 electronic steps
    - only one ionic step
  - "The maximum number of steps has been reached."
- cell shape changes drastically (due to no symmetry?)
  - we've not yet attempted replacing vc relax with atomic relax in the pipeline

# Run DB

## Run Storage and Parallelization Technical Points

- 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
  - may enable improved job parallelization
  - enables more detailed data management