1 Reusing the data

That data is human readable - and machine addressable

We can extract and reuse the data from the original document.

```
1  (remove-if-not (lambda (x) (string= "LDA" (nth 2 x))) data)
```

TiO_2	rutile	LDA	-2801.64	30.58	259.47
TiO_2	anatase	LDA	-2802.73	33.62	187.4
TiO_2	brookite	LDA	-2803.26	31.56	238.06
TiO_2	columbite	LDA	-2803.53	30.0	246.07
TiO_2	pyrite	LDA	-2748.35	27.98	301.15
TiO_2	fluorite	LDA	-2747.3	26.74	316.43

If you prefer Python, no problem. Here we get the anatase data:

```
1  return [x for x in data if x[1] == 'anatase']
```

TiO_2	anatase	LDA	-2802.73	33.62	187.4
TiO_2	anatase	AM05	-2741.12	34.33	178.26
TiO_2	anatase	PBEsol	-2763.61	34.25	178.71
TiO_2	anatase	PBE	-2781.16	35.13	171.42

We can do analysis

```python
1  import json
2  import matplotlib.pyplot as plt
3  from ase.utils.eos import EquationOfState
4  with open('supporting-information.json', 'r') as f:
5      d = json.loads(f.read())
6
7  BO2 = 'VO2'
8  polymorph = 'pyrite'
9  xc = 'LDA'
10
11 volumes = [entry['data']['volume'] for entry in
12           d[BO2][polymorph][xc]['EOS']['calculations']]
13 energies =  [entry['data']['total_energy'] for entry in
14              d[BO2][polymorph][xc]['EOS']['calculations']]
15
16 # Plotting EOS
17 plt.plot(volumes, energies)
18 plt.xlabel('Volume ($3$)')
19 plt.ylabel('Energy (eV)')
20 org.figure(plt.savefig('eos.png'), caption='VO2 pyrite EOS for the LDA functional.')
```

```
(browse-url(org-html-export-to-html))
(org-open-file(org-latex-export-to-pdf))
```