Examples of effective data sharing in scientific publishing

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language: sh

Listing 3: Shell command to print the contents of the INCAR to the console.

```
cat INCAR
```

```
PREC = Normal

ISIF = 2

IBRION = 2

NBANDS = 156

ENCUT = 450.0

NSW = 30
```

language: python

Listing 4: Python script to read the POTCAR file information for a specific calculation.

```
import json
import numpy as np

with open('data.json', 'rb') as f:
    d = json.loads(f.read())

calc = d['results']['HPd']['cln'][0]

print 'POTCARS:'
for sym, potcar, githash in calc['potcar']:
    print(sym, potcar, githash)
```

```
POTCARS:

(u'H', u'potpaw_PBE/H/POTCAR', u'fbc0773b08b32f553234b0b50cc6ad6f5085c816')

(u'Pd', u'potpaw_PBE/Pd/POTCAR', u'abec334aaffe253d3b9fb835c3a06cba6c014023')
```

language: python

Listing 5: Python script to read the other calculation parameters such as k-point sampling, and exchange-correlation functional.

```
import json
import numpy as np

with open('data.json', 'rb') as f:
    d = json.loads(f.read())

calc = d['results']['HPd']['cln'][0]

print 'OTHER INPUT:'
for key, val in calc['input'].items():
    print('{0} = {1}'.format(key, val))
```

```
OTHER INPUT:

kpts = [10, 10, 1]

reciprocal = False

xc = PBE

kpts_nintersections = None

setups = {}

txt = -

gamma = False
```