Materials Project Querying Tool

A postdoc programming challenge: Query the materials project for a given material, count all returned entries and give the ground state material's id.

Getting Started

Run test:

Run the test as follows with `<API_KEY>` replaced by user API key:

```
python3 test_querier.py <API_KEY>
```

Run the main code:

run the main code as follows with `<material>` replaced by the target material's chemical formula , e.g. "Fe2O3":

```
python3 query-mp-database.py <API_KEY> <material>
```

for help

```
python3 query-mp-database.py -h
```

options:

-p : for plotting the results

Example:

input:

```
python3 query-mp-database.py <API_KEY> Fe2O3 -p
```

output:

```
+---------------+-------------------+
| material_id   |   energy_per_atom |
|---------------+-------------------|
| mp-716814     |          -6.18966 |
| mp-609465     |          -6.2578  |
| mvc-12005     |          -6.47026 |
| mp-705773     |          -6.52392 |
| mp-705547     |          -6.54611 |
| mp-777192     |          -6.57339 |
| mp-542309     |          -6.61652 |
| mp-715276     |          -6.66052 |
| mp-686969     |          -6.67518 |
| mp-628327     |          -6.67988 |
| mp-24972      |          -6.71653 |
| mp-715572     |          -6.71684 |
+---------------+-------------------+
12 entries found for query: Fe2O3
Most stable material: mp-715572 (-6.716840 eV/atom)
```

plot:

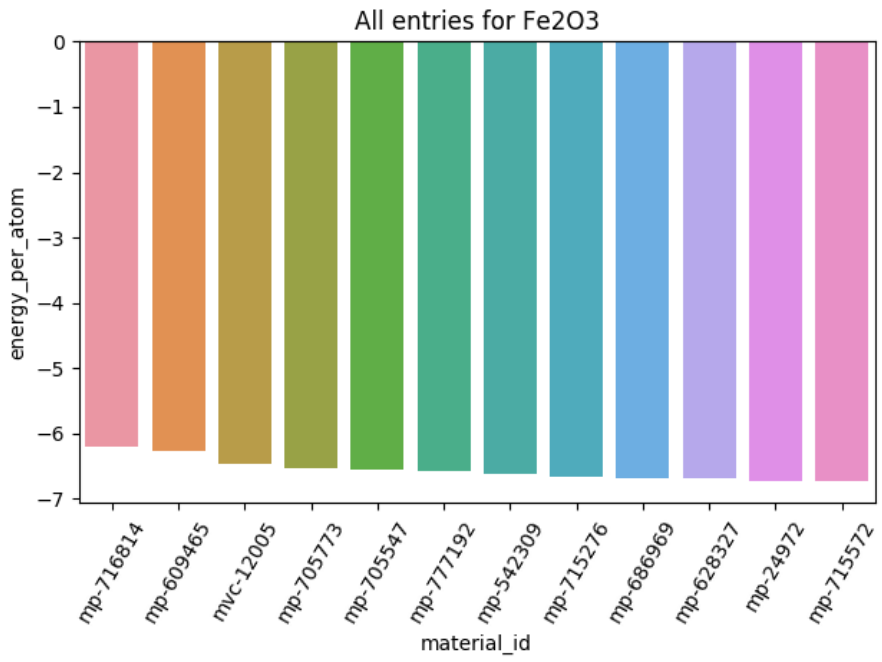

Figure 1: Results

Prerequisites

- python 3.6
- pymatgen
- numpy
- matplotlib
- seaborn
- pandas
- tabulate
- unittest
- requests

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