What are the *httk* and the *omdb*? And, what can they do for YOU?

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Overview

The High-Throughput Toolkit (*httk*)

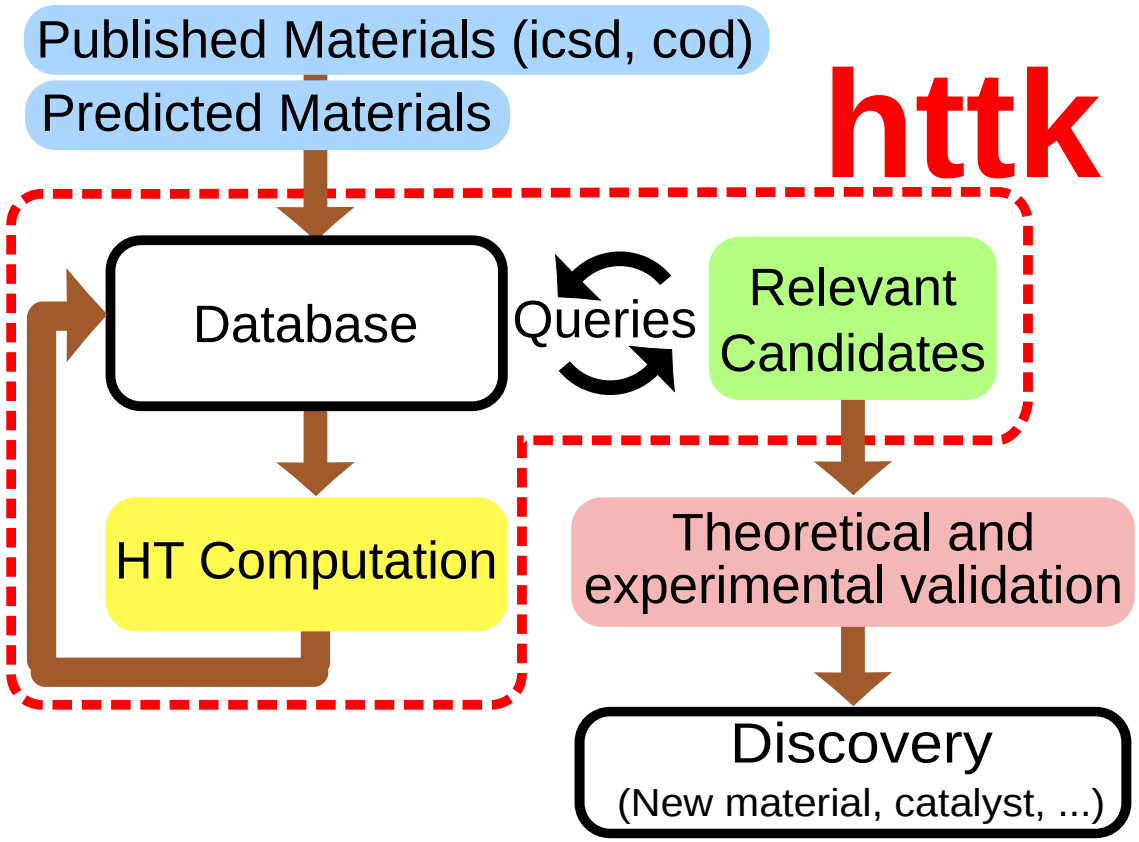
- A toolkit for preparing and running calculations, analyzing the result, store them in a global and/or in a personalized database.
- The primary focus is automatization: run with as little human intervention as possible.
- *Crucial* for large datasets; *convenient* for smaller projects!
- Intended to expand beyond atomistic calculations, but those are our primary focus for now.

The Open Materials Database (omdb)

- A central collection of computational data where we store our results.
- You can, if you want, submit results there as well.
- Easily interacts with *httk*; built using *httk*.

Database-centric High-Throughput

The *httk* is an independent implementation of the Database-centric high-throughput methodology pioneered by G. Ceder, and others.



See: A. Jain, G. Hautier, C. J. Moore, S. P. Ong, C. C. Fischer, T. Mueller, K. A. Persson, G. Ceder, Comp. Mat. Sci. **50**, 2295 (2011).

Overview

Components:

- The *httk* python library:
  - Handling crystal structures.
  - Prepare calculations to be run.
  - Storage, retrieval, search and analysis of data in database.

- The *httk* scripts:
  - Handling large sets of computer runs.
  - Scripting that allow advanced multi-stage runs to be run on clusters with limited walltime.
  - Managing ongoing runs across many supercomputers.
  - Easy submission of results to *omdb*.

Overview

Why not extend existing libraries (ASE, pymatgen, etc.) instead?

- Different core design choices
  - Database interaction as easy as possible; python objects can be stored, searched, retrieved; mixing different databases.
  - Preserves numbers exactly (fractions instead of floating point), helps a lot with crystal geometry and database interaction.
- Different attitude to dependencies
  - No libraries outside standard python needed to get *httk* up and running. Not even numpy or scipy.
  - Other libraries can be/are called when needed.
  - *httk* goes out of its way to help you load the library you want from e.g. odd locations (helpful to, e.g., avoid old system-wide version)
- Instead, *httk* is compatible / interacts with those libraries; i.e., you can translate between ASE, pymatgen, etc., and use their features interchangeably.

Examples

A few programming examples for atomistic computation will follow.

(This is a more technical part of this presentation)

Examples: Structures

Very easy to load a cif file, or poscar, etc.:

```
import httk

struct = httk.load("example.cif")

print("Formula:", struct.formula)
print("Volume", float(struct.uc_volume))
print("Assignments", struct.uc_formula_symbols)
print("Counts:", struct.uc_counts)
print("Coords", struct.uc_reduced_coords)
```

Output:

```
('Formula:', 'BO2Tl')
('Volume', 509.24213999999984)
('Assignments', ['B', 'O', 'Tl'])
('Counts:', [8, 16, 8])
('Coords', FracVector(((1350, 4550, 4250), ..., ,10000)))
```

Examples: Structure

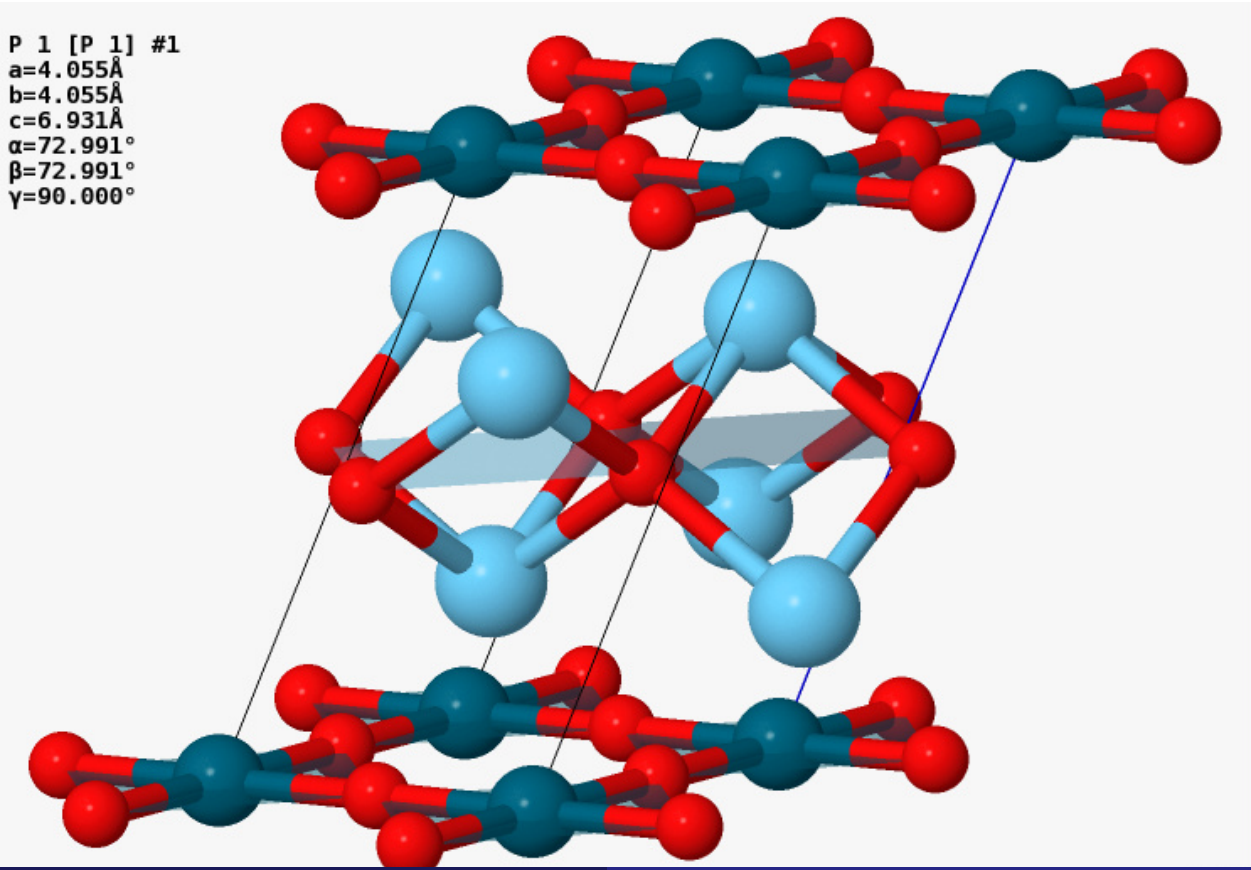
Of course one can also create and modify structures directly in code:

```
from httk.atomistic import Structure

cell = [[1.0, 0.0, 0.0],
        [0.0, 1.0, 0.0],
        [0.0, 0.0, 1.0]]

coordgroups = [[
                   [0.5, 0.5, 0.5]
                ],[
                   [0.0, 0.0, 0.0]
                ],[
                   [0.5, 0.0, 0.0],[0.0, 0.5, 0.0],[0.0, 0.0, 0.5]
               ]]

assignments = ['Pb','Ti','O']
volume=62.79
struct = Structure.create(uc_cell=cell,
            uc_reduced_coordgroups=coordgroups,
            assignments=assignments,
            uc_volume=volume)
```

Examples: Visualization

Easy visualization using, e.g., jmol

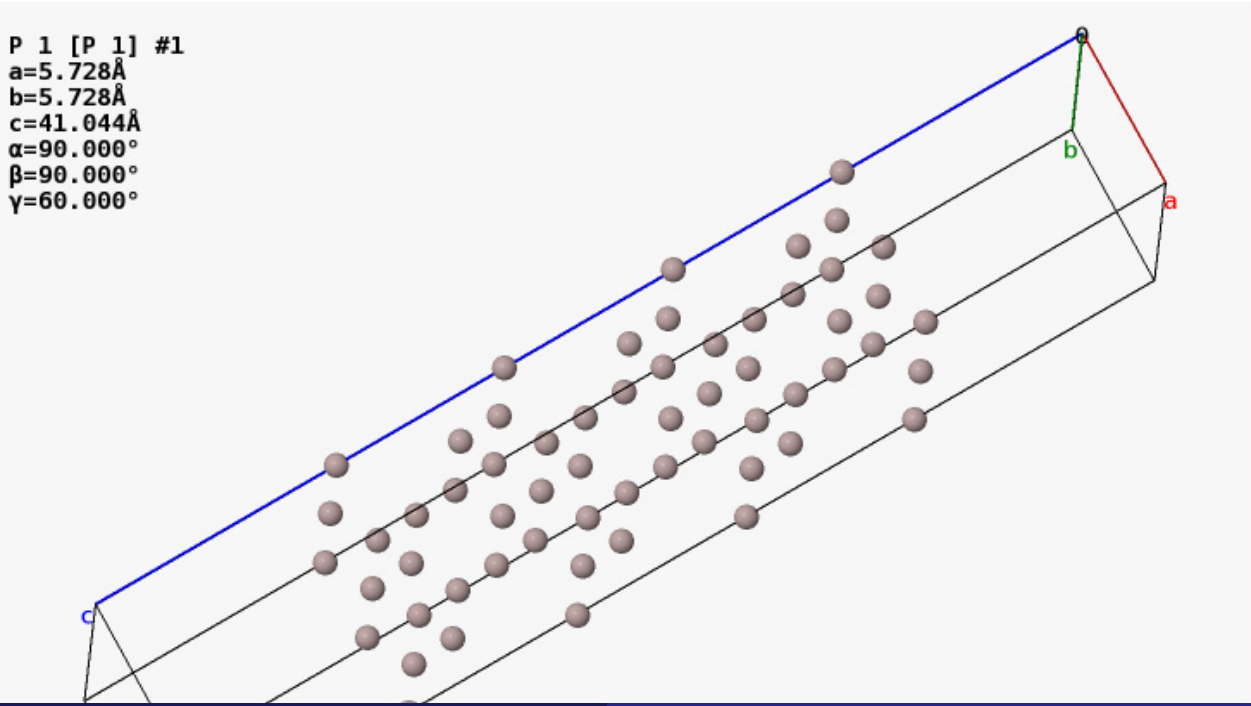
```
import httk
import httk.atomistic.vis

struct = httk.load("POSCAR")
struct.vis.show()
```



Examples: External libraries

Easy interaction with other useful libraries and software, e.g., ASE:
(Present bindings: ASE, aflow, cif2cell, isotropy, jmol, pymatgen, platon, gulp)

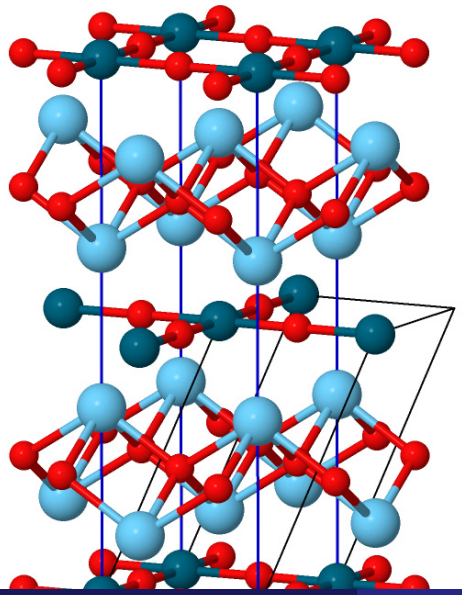
```
from httk.atomistic import Structure
import httk.atomistic.vis
import httk.external.ase_glue
import ase.lattice.surface

slab = ase.lattice.surface.fcc111('Al', size=(2,2,10), vacuum=10.0)
struct = Structure.ase.from_Atoms(slab)
struct.vis.show()
```

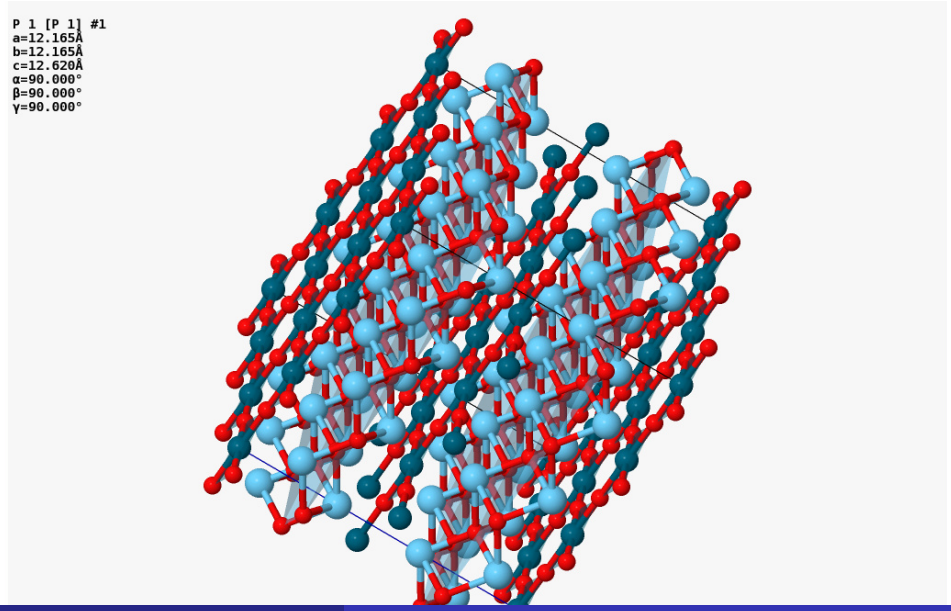


Examples: Supercells

Build supercells, find orthogonal and cubic ones:

```
import httk
import httk.atomistic.vis

struct = httk.load("POSCAR")
supercell1 = struct.build_supercell([[2,0,0],[0,2,0],[0,0,1]])
supercell1.vis.show()
supercell2 = struct.build_orthogonal_supercell(tolerance=20)
supercell2.vis.show()
supercell3 = struct.build_cubic_supercell(tolerance=20)
supercell3.vis.show()
```



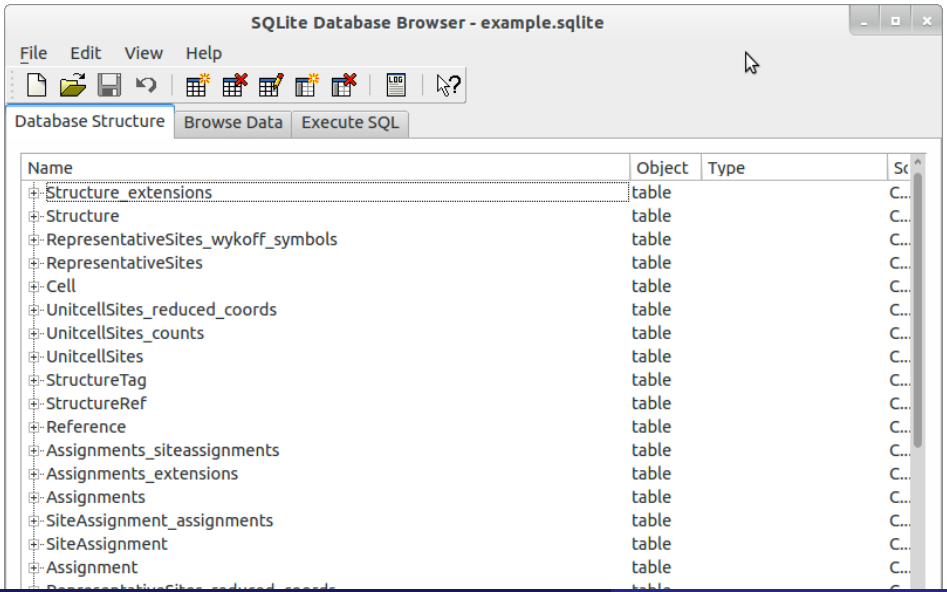


Examples: Database

Store data in a local relational database (sqlite):

```
import httk
import httk.db

backend = httk.db.backend.Sqlite('example.sqlite')
store = httk.db.store.SqlStore(backend)

struct = httk.load('example.cif')
store.save(struct)
```

```
user@computer:> sqlitebrowser example.sqlite
```



Examples: Database

Search in your local database:

```
import httk
from httk.atomistic import Structure
import httk.db

backend = httk.db.backend.Sqlite('example.sqlite')
store = httk.db.store.SqlStore(backend)

search = store.searcher()
search_struct = search.variable(Structure)
search.add( search_struct.uc_nbr_atoms < 40 )

search.output(search_struct,'structure')

for match, header in search:
    struct = match[0]
    print("Found:",struct.formula)
```

Output:

```
('Found:','ZnO2')
```

Examples: Computations

Setup a simple VASP calculation to run manually:

```
import httk
import httk.iface.vasp_if

poscarspath="/path/to/your/poscars/POT_GGA_PAW_PBE/"

struct = httk.load("example.cif")

httk.iface.vasp_if.prepare_single_run("Run", struct,
     template='t:vasp/single/static', poscarspath=poscarspath)
```

```
user@computer:> cd Run
user@computer:> vasp
```

Output:

```
 running on    1 nodes
 distr:  one band on    1 nodes,    1 groups
 vasp.5.2.12 11Nov11 complex

 POSCAR found type information on POSCAR  Ti N
 POSCAR found :  2 types and       2 ions
```

Examples: Computations

Generate a big batch of computations:

```
import httk, httk.task, httk.db
from httk.atomistic import Structure

backend = httk.db.backend.Sqlite('tutorial.sqlite')
store = httk.db.store.SqlStore(backend)

search = store.searcher()
search_struct = search.variable(Structure)
search.add_all(search_struct.formula_symbols.is_in('O','Ca','Ti'))
search.output(search_struct,'structure')

for match, header in search:
  struct = match[0]
  httk.task.create_batch_task('Runs','/vasp/batch/relax',
    {"structure":struct})
```

Examples: Computations

Run the batch of computations on a supercomputer ('kappa'):

```
user@computer:> httk-project-setup example_project
user@computer:> httk-computer-setup ssh-slurm kappa
user@computer:> httk-computer-install kappa
```

```
user@computer:> httk-tasks-send-to-computer kappa Runs/
user@computer:> httk-tasks-start-taskmanager kappa
```

```
user@computer:> httk-tasks-status kappa
```

```
user@computer:> httk-tasks-receive-from-computer kappa Runs/
```

Examples: Computations

Read results back into database

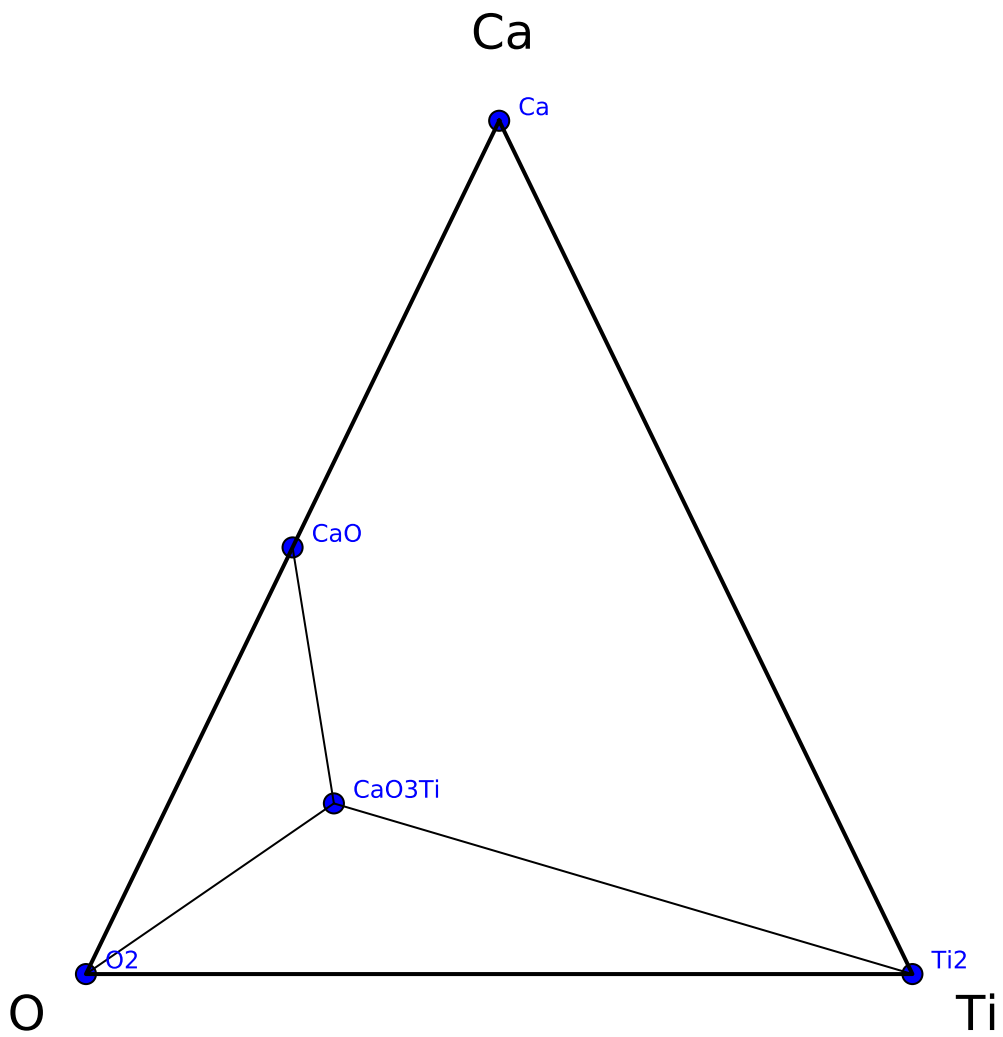
```
import httk, httk.db, httk.task, os
from httk.atomistic.results import Result_TotalEnergyResult

backend = httk.db.backend.Sqlite('example.sqlite')
store = httk.db.store.SqlStore(backend)

reader = httk.task.reader('./','Runs/')

for rundir, computation in reader:
    struct = httk.load(os.path.join(rundir,"CONTCAR"))
    outcar = httk.iface.vasp_if.read_outcar(os.path.join(rundir,"
        OUTCAR.cleaned.relax2"))
    total_energy_result = Result_TotalEnergyResult(computation,
        struct, float(outcar.final_energy))
    store.save(total_energy_result)
```

Examples: Computations

Draw a phase diagram from your stored batch runs

```
import httk, httk.db, httk.task, httk.atomistic.vis
from httk.atomistic import Structure, StructurePhaseDiagram
from httk.atomistic.results import Result_TotalEnergyResult

backend = httk.db.backend.Sqlite('example.sqlite')
store = httk.db.store.SqlStore(backend)
search = store.searcher()
search_total_energy = search.variable(Result_TotalEnergyResult)
search_struct = search.variable(Structure)
search.add(search_total_energy.structure == search_struct)
search.add_all(search_struct.formula_symbols.is_in('O','Ca','Ti'))
search.output(search_total_energy,'total_energy_result')

structures, energies = [],[]
for match, header in search:
    total_energy_result = match[0]
    structures += [total_energy_result.structure]
    energies += [total_energy_result.total_energy]

pd = StructurePhaseDiagram.create(structures,energies)
pd.vis.show(debug=True)
```

Examples: Computations



Note: phase-diagram support in httk does not yet draw *all* phase lines.

Examples: Computations

It is easy to put your own data in the database

```
import httk, httk.db
from httk.atomistic import Structure

class StructureIsEdible(httk.HttkObject):
    @httk.httk_typed_init({'structure':Structure,
                           'is_edible':bool})
    def __init__(self, structure, is_edible):
        self.structure = structure
        self.is_edible = is_edible

backend = httk.db.backend.Sqlite('example.sqlite')
store = httk.db.store.SqlStore(backend)

tablesalt = httk.load('NaCl.cif')
arsenic = httk.load('As.cif')

edible = StructureIsEdible(tablesalt,True)
store.save(edible)
edible = StructureIsEdible(arsenic,False)
store.save(edible)
```

Submit results to the global database

Submit to central database

```
user@computer:> httk-project-submit
```

Note:

- Will verify very carefully that you actually mean to make your data publicly available on the web via *omdb*.
- Your files are signed by a private key; you can always be identified as the 'owner' of these files.
- You can change/add reference information after submission by editing ht.project/references and running httk-project-submit-update-references
- You can withdraw your data at a later point with httk-project-submit-widthdraw

Note: when you run `httk-project-setup` a directory `ht.project` is created to identify *this* project. You can copy the project directory everywhere you have files relating to this project. You can then run `httk-project-submit` in each such directory, and the files are aggregated on our servers.

Open Materials Database

Open Materials Datab ×

openmaterialsdb.se/index.php?compound_cid=1050#tab_results

Open *Materials Database* (beta)

Present database:
Materials: 9617
Computations: 2787

Materials | Computations | Advanced | Manual Query | Help | About

Search for Materials that Match Criteria

Magnesium

submit

(Usage help: 'NaCl' or 'Sodium Chloride' searches for specifically NaCl. Use '*' as a wildcard. '+Na +Cl' searches for anything with Na and Cl species. More help on our help page.)

Data on material: Mg3O8P2 (1050)

General Data

- Formula: Mg3O8P2
- Name: Magnesium phosphate
- Download (unrelaxed) structure as: POSCAR
- Abstract formula: A2B3C8
- Element count: 3
- Spacegroup number: 14

Results related to this material

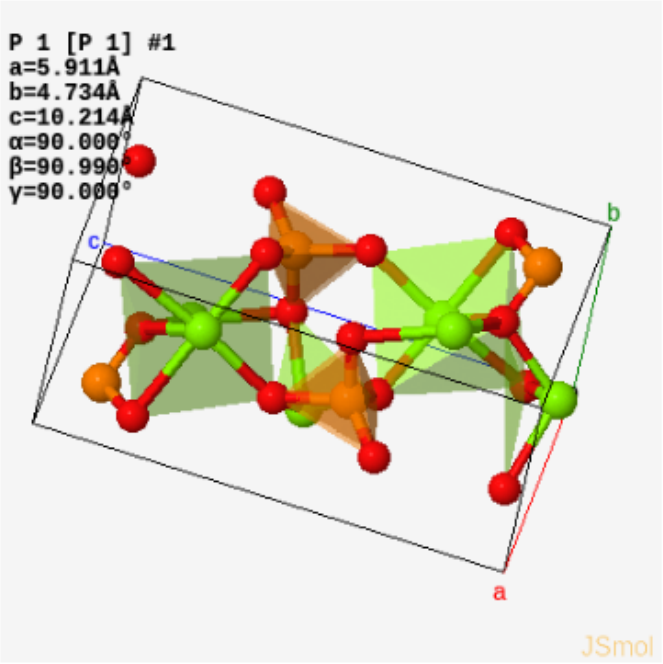
#	TableName	Table_id
1	FakeEnergy	823

Computations related to this material

#	Computation_id	computation_date	added_date	description	relation
1	52	2014-07-27T20:17:35.173722	2014-07-27T20:17:35.173722	Extract compounds from imported structures	Identified as new compound

References for this material

#	reference
1	Berthet, G et al., Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik,Kristallchemie (-144,1977) 136, 98-105 (1972)



Operate on Data in Open Materials Database

Operate directly on data present in the open materials database:
(Not in present version; will be in next.)

```
import httk, httk.db
from httk.atomistic import Structure

store = httk.db.open_materials_database_store

search = store.searcher()
search_struct = search.variable(Structure)
search.add_all(search_struct.formula_symbols.is_in('O','Ca','Ti'))
search.output(search_struct,'structure')

for match, header in search:
  struct = match[0]
  httk.task.create_batch_task('Runs','template',
    {"structure":struct})
```

Installation

Easy to install

Linux / Unix / Mac OS X / Cygwin:

```
user@computer:> mkdir ~/bin/python
user@computer:> cd ~/bin/python
user@computer:> curl -O http://httk.openmaterialsdb.se/downloads/
    httk-latest.tgz
user@computer:> tar -zxvf httk-latest.tgz
user@computer:> ls
  httk-1.0.0  httk-latest.tgz
user@computer:> ln -f -s httk-1.0.0 httk-latest
user@computer:> source ~/bin/python/httk-latest/setup.shell
```

Put the last statement in your .bashrc / .cshrc to always set the paths up correctly.

Concluding remarks

- The High-Throughput Toolkit (*httk*) is a framework for easy automatization of computational projects. It helps with setup, execution, storage and search.
- A framework like this is *crucial* for projects that work with large datasets, but also *convenient* for smaller projects.
- For our own calculations, we store them at `openmaterialsdb.se`; you can also submit your results there if you want (with your papers cited and linked).

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