CatOGM

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1 Bulk Fingerprint Generator

This module/class is designed to calculate bulk fingerprints for regular bulk structures. In the following, a simple example is shown how to use it.

1.1 For a single bulk structure

```
from catogm.fingerprint.bulk_fp import Bulk_fp_generator
from ase.build import bulk

atoms1 = bulk('Pd', cubic=True)
atoms1.set_chemical_symbols('Pd3Pt')


convoluted_params = features = ['atomic_number',
                                'atomic_radius',
                                'atomic_volume',
                                'atomic_weight',
                                'boiling_point',
                                'covalent_radius_cordero',
                                'dipole_polarizability',
                                'electron_affinity',
                                'en_pauling',
                                'en_allen',
                                'en_ghosh',
                                'evaporation_heat',
                                'fusion_heat',
                                'group_id',
                                'period',
                                'heat_of_formation',
                                'melting_point',
                                'metallic_radius',
                                'specific_heat',
                                'thermal_conductivity',
                                'vdw_radius',
                                'd-band_center',
                                'd-band_width',
                                'd-band_skewness',
                                'd-band_kurtosis']
```

```
33
34  nonc_params = ['stoichiometry',
35                 'lattice_constant_a',
36                 'lattice_constant_c']
37
38  bfp_gen = Bulk_fp_generator()
39
40  print('Bulk fingerprints:\n')
41  fp_names = bfp_gen.return_fp_names(convoluted_params, nonc_params, io_mode='list')
42  for i in fp_names:
43      print(i)
44
45  print('\nComputed bulk fingerprints are:\n')
46  print(bfp_gen.return_fp(atoms1, convoluted_params, nonc_params))
```

```
Bulk fingerprints:

stoichiometry
lattice_constant_a
lattice_constant_c
atomic_number_0
atomic_number_1
atomic_radius_0
atomic_radius_1
atomic_volume_0
atomic_volume_1
atomic_weight_0
atomic_weight_1
boiling_point_0
boiling_point_1
covalent_radius_cordero_0
covalent_radius_cordero_1
dipole_polarizability_0
dipole_polarizability_1
electron_affinity_0
electron_affinity_1
en_pauling_0
en_pauling_1
en_allen_0
en_allen_1
en_ghosh_0
en_ghosh_1
evaporation_heat_0
evaporation_heat_1
```

```
fusion_heat_0
fusion_heat_1
group_id_0
group_id_1
period_0
period_1
heat_of_formation_0
heat_of_formation_1
melting_point_0
melting_point_1
metallic_radius_0
metallic_radius_1
specific_heat_0
specific_heat_1
thermal_conductivity_0
thermal_conductivity_1
vdw_radius_0
vdw_radius_1
d-band_center_0
d-band_center_1
d-band_width_0
d-band_width_1
d-band_skewness_0
d-band_skewness_1
d-band_kurtosis_0
d-band_kurtosis_1

Computed bulk fingerprints are:

[7.90000000e-01 3.89000000e+00 3.89000000e+00 1.24320000e+04
 1.36896000e+05 7.56280000e+04 9.07488000e+05 3.20440000e+02
 3.84480000e+03 7.20334163e+04 7.70065336e+05 5.17557070e+07
 6.15404856e+08 7.64590000e+04 9.17400000e+05 5.00800000e+03
 5.83680000e+04 5.47591600e+00 3.62827200e+01 1.93600000e+01
 2.32320000e+02 3.68418412e+02 4.41412618e+03 1.28234597e-01
 1.38590593e+00 6.36945280e+05 7.52903424e+06 1.36515040e+03
 1.61366400e+04 4.00000000e+02 4.80000000e+03 1.11000000e+02
 1.32000000e+03 7.45499170e+05 8.51688432e+06 1.41739000e+07
 1.69506000e+08 6.60520000e+04 7.92576000e+05 1.96297000e-01
 2.20771200e+00 2.05922800e+04 2.47106880e+05 1.77669000e+05
```

```
2.13192000e+06 2.15572812e+01 2.56278228e+02 7.65027472e+02
8.81334181e+03 7.17384783e+03 8.60253749e+04 1.58217274e+07
1.71200649e+08]
```

1.2 For a list of bulk structures

```python
from catogm.fingerprint.bulk_fp import Bulk_fp_generator
from ase.build import bulk

atoms1 = bulk('Pd', cubic=True)
atoms2 = bulk('Pd', cubic=True)
atoms2.set_chemical_symbols('Pd3Pt')
atoms3 = bulk('Pd', cubic=True)
atoms3.set_chemical_symbols('Pd2Pt2')

convoluted_params = features = ['atomic_number',
                                'atomic_radius',
                                'atomic_volume',
                                'atomic_weight',
                                'boiling_point',
                                'covalent_radius_cordero',
                                'dipole_polarizability',
                                'electron_affinity',
                                'en_pauling',
                                'en_allen',
                                'en_ghosh',
                                'evaporation_heat',
                                'fusion_heat',
                                'group_id',
                                'period',
                                'heat_of_formation',
                                'melting_point',
                                'metallic_radius',
                                'specific_heat',
                                'thermal_conductivity',
                                'vdw_radius',
                                'd-band_center',
                                'd-band_width',
                                'd-band_skewness',
                                'd-band_kurtosis']

nonc_params = ['stoichiometry',
               'lattice_constant_a',
               'lattice_constant_c']

bfp_gen = Bulk_fp_generator()

print('Bulk fingerprints:\n')
fp_names = bfp_gen.return_fp_names(convoluted_params, nonc_params, io_mode='list')
for i in fp_names:
    print(i)

list_atoms = [atoms1, atoms2, atoms3]
print('\nComputed bulk fingerprints are:\n')
```

```
49 print(bfp_gen.return_fp(list_atoms, convoluted_params, nonc_params))
```

```
Bulk fingerprints:

stoichiometry
lattice_constant_a
lattice_constant_c
atomic_number_0
atomic_number_1
atomic_radius_0
atomic_radius_1
atomic_volume_0
atomic_volume_1
atomic_weight_0
atomic_weight_1
boiling_point_0
boiling_point_1
covalent_radius_cordero_0
covalent_radius_cordero_1
dipole_polarizability_0
dipole_polarizability_1
electron_affinity_0
electron_affinity_1
en_pauling_0
en_pauling_1
en_allen_0
en_allen_1
en_ghosh_0
en_ghosh_1
evaporation_heat_0
evaporation_heat_1
fusion_heat_0
fusion_heat_1
group_id_0
group_id_1
period_0
period_1
heat_of_formation_0
heat_of_formation_1
melting_point_0
```

```
melting_point_1
metallic_radius_0
metallic_radius_1
specific_heat_0
specific_heat_1
thermal_conductivity_0
thermal_conductivity_1
vdw_radius_0
vdw_radius_1
d-band_center_0
d-band_center_1
d-band_width_0
d-band_width_1
d-band_skewness_0
d-band_skewness_1
d-band_kurtosis_0
d-band_kurtosis_1

Computed bulk fingerprints are:

[[1.00000000e+00 3.89000000e+00 3.89000000e+00 8.46400000e+03
  1.01568000e+05 7.50760000e+04 9.00912000e+05 3.16840000e+02
  3.80208000e+03 4.53008656e+04 5.43610387e+05 4.65942760e+07
  5.59131312e+08 7.72840000e+04 9.27408000e+05 4.09600000e+03
  4.91520000e+04 1.26337600e+00 1.51605120e+01 1.93600000e+01
  2.32320000e+02 3.53590416e+02 4.24308499e+03 8.29757982e-02
  9.95709579e-01 5.54727040e+05 6.65672448e+06 1.18887040e+03
  1.42664448e+04 4.00000000e+02 4.80000000e+03 1.00000000e+02
  1.20000000e+03 5.67310240e+05 6.80772288e+06 1.33225000e+07
  1.59870000e+08 6.55360000e+04 7.86432000e+05 2.38144000e-01
  2.85772800e+00 2.06209600e+04 2.47451520e+05 1.76400000e+05
  2.11680000e+06 1.93838208e+01 2.32605850e+02 5.99088189e+02
  7.18905827e+03 7.36191269e+03 8.83429523e+04 1.98180439e+07
  2.37816527e+08]
 [7.90000000e-01 3.89000000e+00 3.89000000e+00 1.24320000e+04
  1.36896000e+05 7.56280000e+04 9.07488000e+05 3.20440000e+02
  3.84480000e+03 7.20334163e+04 7.70065336e+05 5.17557070e+07
  6.15404856e+08 7.64590000e+04 9.17400000e+05 5.00800000e+03
  5.83680000e+04 5.47591600e+00 3.62827200e+01 1.93600000e+01
  2.32320000e+02 3.68418412e+02 4.41412618e+03 1.28234597e-01
```

```
  1.38590593e+00 6.36945280e+05 7.52903424e+06 1.36515040e+03
  1.61366400e+04 4.00000000e+02 4.80000000e+03 1.11000000e+02
  1.32000000e+03 7.45499170e+05 8.51688432e+06 1.41739000e+07
  1.69506000e+08 6.60520000e+04 7.92576000e+05 1.96297000e-01
  2.20771200e+00 2.05922800e+04 2.47106880e+05 1.77669000e+05
  2.13192000e+06 2.15572812e+01 2.56278228e+02 7.65027472e+02
  8.81334181e+03 7.17384783e+03 8.60253749e+04 1.58217274e+07
  1.71200649e+08]
 [7.10000000e-01 3.89000000e+00 3.89000000e+00 1.64000000e+04
  1.80416000e+05 7.61800000e+04 9.14096000e+05 3.24040000e+02
  3.88784000e+03 9.87659669e+04 1.05941072e+06 5.69171380e+07
  6.75454152e+08 7.56340000e+04 9.07464000e+05 5.92000000e+03
  6.87360000e+04 9.68845600e+00 7.70237760e+01 1.93600000e+01
  2.32320000e+02 3.83246408e+02 4.58976387e+03 1.73493395e-01
  1.87804176e+00 7.19163520e+05 8.47755008e+06 1.54143040e+03
  1.81702784e+04 4.00000000e+02 4.80000000e+03 1.22000000e+02
  1.44800000e+03 9.23688100e+05 1.05121162e+07 1.50253000e+07
  1.79529200e+08 6.65680000e+04 7.98752000e+05 1.54450000e-01
  1.65626400e+00 2.05636000e+04 2.46762560e+05 1.78938000e+05
  2.14711200e+06 2.37307416e+01 2.81556705e+02 9.30966754e+02
  1.06822839e+04 6.98578296e+03 8.37483302e+04 1.18254108e+07
  1.17024824e+08]]
```

2 Slab Fingerprint Generator

This module/class is designed to calculate slab fingerprints for regular bulk structures. In the following, we show a simple example on how to use it.

2.1 For a single slab structure

```python
from catogm.fingerprint.slab_fp import Slab_fp_generator
from ase.build import fcc111

slab = fcc111('Al', size=(2,2,3), vacuum=10.0)

convoluted_params = features = ['atomic_number',
                                'atomic_radius',
                                'atomic_volume',
                                'atomic_weight',
                                'boiling_point',
                                'covalent_radius_cordero',
                                'dipole_polarizability',
                                'electron_affinity',
```

```
                                    'en_pauling',
                                    'en_allen',
                                    'en_ghosh',
                                    'evaporation_heat',
                                    'fusion_heat',
                                    'group_id',
                                    'period',
                                    'heat_of_formation',
                                    'melting_point',
                                    'metallic_radius',
                                    'specific_heat',
                                    'thermal_conductivity',
                                    'vdw_radius',
                                    'd-band_center',
                                    'd-band_width',
                                    'd-band_skewness',
                                    'd-band_kurtosis']


sfp_gen = Slab_fp_generator()

print('Slab fingerprints:\n')
fp_names = sfp_gen.return_fp_names(convoluted_params)
for i in fp_names:
    print(i)

print('\nComputed slab fingerprints are:\n')
print(sfp_gen.return_fp(slab, convoluted_params))
```

```
Slab fingerprints:

atomic_number_0
atomic_number_1
atomic_radius_0
atomic_radius_1
atomic_volume_0
atomic_volume_1
atomic_weight_0
atomic_weight_1
boiling_point_0
boiling_point_1
covalent_radius_cordero_0
covalent_radius_cordero_1
dipole_polarizability_0
dipole_polarizability_1
electron_affinity_0
electron_affinity_1
en_pauling_0
```

```
en_pauling_1
en_allen_0
en_allen_1
en_ghosh_0
en_ghosh_1
evaporation_heat_0
evaporation_heat_1
fusion_heat_0
fusion_heat_1
group_id_0
group_id_1
period_0
period_1
heat_of_formation_0
heat_of_formation_1
melting_point_0
melting_point_1
metallic_radius_0
metallic_radius_1
specific_heat_0
specific_heat_1
thermal_conductivity_0
thermal_conductivity_1
vdw_radius_0
vdw_radius_1
d-band_center_0
d-band_center_1
d-band_width_0
d-band_width_1
d-band_skewness_0
d-band_skewness_1
d-band_kurtosis_0
d-band_kurtosis_1

Computed slab fingerprints are:

[2.02800000e+03 2.02800000e+04 2.45388000e+05 2.45388000e+06
 1.20000000e+03 1.20000000e+04 8.73604104e+03 8.73604104e+04
 9.00912000e+07 9.00912000e+08 1.75692000e+05 1.75692000e+06
 2.53920000e+04 2.53920000e+05 2.24810171e+00 2.24810171e+01
```

```
 3.11052000e+01 3.11052000e+02 1.09191025e+03 1.09191025e+04
 2.70280873e-01 2.70280873e+00 9.68553720e+05 9.68553720e+06
 1.38675000e+03 1.38675000e+04 2.02800000e+03 2.02800000e+04
 1.08000000e+02 1.08000000e+03 1.31393772e+06 1.31393772e+07
 1.04570670e+07 1.04570670e+08 1.87500000e+05 1.87500000e+06
 9.72000000e+00 9.72000000e+01 6.74028000e+05 6.74028000e+06
 4.06272000e+05 4.06272000e+06            nan            nan
            nan            nan            nan            nan
            nan            nan]
```

2.2 For a list of slab structures

```
from catogm.fingerprint.slab_fp import Slab_fp_generator
from ase.build import fcc111

slab = fcc111('Al', size=(2,2,3), vacuum=10.0)
slab1 = fcc111('Pd', size=(2,2,3), vacuum=10.0)
slab2 = fcc111('Pt', size=(2,2,3), vacuum=10.0)

convoluted_params = features = ['atomic_number',
                                'atomic_radius',
                                'atomic_volume',
                                'atomic_weight',
                                'boiling_point',
                                'covalent_radius_cordero',
                                'dipole_polarizability',
                                'electron_affinity',
                                'en_pauling',
                                'en_allen',
                                'en_ghosh',
                                'evaporation_heat',
                                'fusion_heat',
                                'group_id',
                                'period',
                                'heat_of_formation',
                                'melting_point',
                                'metallic_radius',
                                'specific_heat',
                                'thermal_conductivity',
                                'vdw_radius',
                                'd-band_center',
                                'd-band_width',
                                'd-band_skewness',
                                'd-band_kurtosis']


sfp_gen = Slab_fp_generator()

list_slabs = [slab, slab1, slab2]


```

```
print('Slab fingerprints:\n')
fp_names = sfp_gen.return_fp_names(convoluted_params)
for i in fp_names:
    print(i)

print('\nComputed slab fingerprints are:\n')
print(sfp_gen.return_fp(list_slabs, convoluted_params))
```

```
Slab fingerprints:

atomic_number_0
atomic_number_1
atomic_radius_0
atomic_radius_1
atomic_volume_0
atomic_volume_1
atomic_weight_0
atomic_weight_1
boiling_point_0
boiling_point_1
covalent_radius_cordero_0
covalent_radius_cordero_1
dipole_polarizability_0
dipole_polarizability_1
electron_affinity_0
electron_affinity_1
en_pauling_0
en_pauling_1
en_allen_0
en_allen_1
en_ghosh_0
en_ghosh_1
evaporation_heat_0
evaporation_heat_1
fusion_heat_0
fusion_heat_1
group_id_0
group_id_1
period_0
period_1
heat_of_formation_0
```

```
heat_of_formation_1
melting_point_0
melting_point_1
metallic_radius_0
metallic_radius_1
specific_heat_0
specific_heat_1
thermal_conductivity_0
thermal_conductivity_1
vdw_radius_0
vdw_radius_1
d-band_center_0
d-band_center_1
d-band_width_0
d-band_width_1
d-band_skewness_0
d-band_skewness_1
d-band_kurtosis_0
d-band_kurtosis_1

Computed slab fingerprints are:

[[2.02800000e+03 2.02800000e+04 2.45388000e+05 2.45388000e+06
  1.20000000e+03 1.20000000e+04 8.73604104e+03 8.73604104e+04
  9.00912000e+07 9.00912000e+08 1.75692000e+05 1.75692000e+06
  2.53920000e+04 2.53920000e+05 2.24810171e+00 2.24810171e+01
  3.11052000e+01 3.11052000e+02 1.09191025e+03 1.09191025e+04
  2.70280873e-01 2.70280873e+00 9.68553720e+05 9.68553720e+06
  1.38675000e+03 1.38675000e+04 2.02800000e+03 2.02800000e+04
  1.08000000e+02 1.08000000e+03 1.31393772e+06 1.31393772e+07
  1.04570670e+07 1.04570670e+08 1.87500000e+05 1.87500000e+06
  9.72000000e+00 9.72000000e+01 6.74028000e+05 6.74028000e+06
  4.06272000e+05 4.06272000e+06            nan            nan
             nan            nan            nan            nan
             nan            nan]
 [2.53920000e+04 2.53920000e+05 2.25228000e+05 2.25228000e+06
  9.50520000e+02 9.50520000e+03 1.35902597e+05 1.35902597e+06
  1.39782828e+08 1.39782828e+09 2.31852000e+05 2.31852000e+06
  1.22880000e+04 1.22880000e+05 3.79012800e+00 3.79012800e+01
  5.80800000e+01 5.80800000e+02 1.06077125e+03 1.06077125e+04
```

```
  2.48927395e-01 2.48927395e+00 1.66418112e+06 1.66418112e+07
  3.56661120e+03 3.56661120e+04 1.20000000e+03 1.20000000e+04
  3.00000000e+02 3.00000000e+03 1.70193072e+06 1.70193072e+07
  3.99675000e+07 3.99675000e+08 1.96608000e+05 1.96608000e+06
  7.14432000e-01 7.14432000e+00 6.18628800e+04 6.18628800e+05
  5.29200000e+05 5.29200000e+06 3.28495738e+01 3.28495738e+02
  5.91455943e+02 5.91455943e+03 8.96168358e+04 8.96168358e+05
  1.73995904e+08 1.73995904e+09]
 [7.30080000e+04 7.30080000e+05 2.31852000e+05 2.31852000e+06
  9.93720000e+02 9.93720000e+03 4.56693205e+05 4.56693205e+06
  2.01720000e+08 2.01720000e+09 2.21952000e+05 2.21952000e+06
  2.32320000e+04 2.32320000e+05 5.43406080e+01 5.43406080e+02
  5.80800000e+01 5.80800000e+02 1.23870720e+03 1.23870720e+04
  7.92032977e-01 7.92032977e+00 2.65080000e+06 2.65080000e+07
  5.68197120e+03 5.68197120e+04 1.20000000e+03 1.20000000e+04
  4.32000000e+02 4.32000000e+03 3.84019788e+06 3.84019788e+07
  5.01843000e+07 5.01843000e+08 2.02800000e+05 2.02800000e+06
  2.12268000e-01 2.12268000e+00 6.15187200e+04 6.15187200e+05
  5.44428000e+05 5.44428000e+06 4.71157525e+01 4.71157525e+02
  8.98448862e+02 8.98448862e+03 9.79101412e+03 9.79101412e+04
  4.46763322e+05 4.46763322e+06]]
```

3 Adsorbate Fingerprint Generation

This class/module is designed to compute the fingerprints for a single adsorbate atoms. However, it can easily be extended to complex adsorbate system.

3.1 For carbon

```python
from catogm.fingerprint.adsorbate_fp import Adsorbate_fp_generator
from ase.atoms import Atoms
from pprint import pprint

atoms1 = Atoms('C')

fp_params = ['atomic_number',
             'atomic_radius',
             'atomic_volume',
             'atomic_weight',
             'boiling_point',
             'covalent_radius_cordero',
             'dipole_polarizability',
```

```
14              'electron_affinity',
15              'en_pauling',
16              'en_allen',
17              'en_ghosh',
18              'evaporation_heat',
19              'fusion_heat',
20              'group_id',
21              'period',
22              'heat_of_formation',
23              'melting_point',
24              'metallic_radius',
25              'specific_heat',
26              'thermal_conductivity',
27              'vdw_radius']
28
29  afp_gen = Adsorbate_fp_generator()
30
31  print('Adsorbate fingerprints:\n')
32  fp_names = afp_gen.return_fp_names(fp_params)
33  for i in fp_names:
34      print(i)
35
36  print('\nComputed adsorbate fingerprints are:\n')
37  fp_list = afp_gen.return_fp_list(atoms1, fp_params)
38  pprint(fp_list)
```

```
Adsorbate fingerprints:

atomic_number
atomic_radius
atomic_volume
atomic_weight
boiling_point
covalent_radius_cordero
dipole_polarizability
electron_affinity
en_pauling
en_allen
en_ghosh
evaporation_heat
fusion_heat
group_id
period
heat_of_formation
melting_point
metallic_radius
specific_heat
```

```
thermal_conductivity
vdw_radius

Computed adsorbate fingerprints are:

[6,
 91.0,
 5.3,
 12.011,
 5100.0,
 73.0,
 20.53,
 1.262119,
 2.55,
 15.05,
 0.22477600000000003,
 nan,
 nan,
 14,
 2,
 716.87,
 3820.0,
 nan,
 0.711,
 1.59,
 170.0]
```

4 Adsorbate-slab Fingerprint Generation

This class/module is designed to compute the fingerprints for properties related to the adsorbate and surrounnding metal environment.

4.1 For carbon adsorbed on Pd slab

```
from catogm.fingerprint.adsorbate_slab_fp import Adsorbate_slab_fp_generator
from ase.build import fcc111
from ase.build import add_adsorbate
from pprint import pprint

slab = fcc111('Pd', size=(2,2,3), vacuum=10.0)
add_adsorbate(slab, 'C', 1.5, 'ontop')
```

```
8
9  ads_metal_params = ['atomic_number',
10                      'atomic_radius',
11                      'atomic_volume',
12                      'atomic_weight',
13                      'boiling_point',
14                      'covalent_radius_cordero',
15                      'dipole_polarizability',
16                      'electron_affinity',
17                      'en_pauling',
18                      'en_allen',
19                      'en_ghosh',
20                      'evaporation_heat',
21                      'fusion_heat',
22                      'group_id',
23                      'period',
24                      'heat_of_formation',
25                      'melting_point',
26                      'metallic_radius',
27                      'specific_heat',
28                      'thermal_conductivity',
29                      'vdw_radius',
30                      'ads_connectivity']
31
32 metal_params = ['d-band_center',
33                 'd-band_width',
34                 'd-band_skewness',
35                 'd-band_kurtosis']
36
37
38 asfp_gen = Adsorbate_slab_fp_generator()
39
40 print('Adsorbate-slab fingerprints:\n')
41 fp_names = asfp_gen.return_fp_names(ads_metal_params, metal_params)
42 for i in fp_names:
43     print(i)
44
45 print('\nComputed adsorbate-slab fingerprints are:\n')
46 pprint(asfp_gen.return_fp_list(slab, ads_metal_params, metal_params))
```

```
Adsorbate-slab fingerprints:

atomic_number
atomic_radius
atomic_volume
atomic_weight
boiling_point
covalent_radius_cordero
dipole_polarizability
electron_affinity
en_pauling
```

```
en_allen
en_ghosh
evaporation_heat
fusion_heat
group_id
period
heat_of_formation
melting_point
metallic_radius
specific_heat
thermal_conductivity
vdw_radius
ads_connectivity
d-band_center
d-band_width
d-band_skewness
d-band_kurtosis

Computed adsorbate-slab fingerprints are:

[276.0,
 12467.0,
 47.17,
 1278.2106199999998,
 17406300.0,
 10147.0,
 656.96,
 0.709310878,
 5.61,
 141.50010000000003,
 0.03237394781760001,
 nan,
 nan,
 140.0,
 10.0,
 269973.242,
 6971500.0,
 nan,
 0.173484,
 114.162,
```

35700.0,
1,
-1.6545284777476137,
7.020540950171534,
-86.41799377922942,
3807.841735270619]