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]
```