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

```
#!/usr/bin/env python
# -*-coding: utf-8 -*-

#bulk_fp_test.py
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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']

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

bfp_gen = Bulk_fp_generator()

print(bfp_gen.return_fp(atoms1, convoluted_params, nonc_params))
print(bfp_gen.return_fp_names(convoluted_params, nonc_params, io_mode='list'))
```