

GAP_6

```
<command_line><![CDATA[ at_file=teach.xyz descriptor_str={soap l_max=14 n_max=14 atom_sigma=0.5 zeta=4 cutoff=5.0
cutoff_transition_width=1.0 delta=1.0 f0=0.0 covariance_type=dot_product sparse_method=kmeans n_sparseX=10000} do_sparse
default_sigma={0.001 0.1 0.1} config_type_sigma={slice_sample:0.0001:0.01:0.01} e0=-9.19483512529700 sparse_jitter=1.0e-6
energy_parameter_name=energy force_parameter_name=force virial_parameter_name=virial config_type_parameter_name=config_type
gp_file=gp.xml sparseX_separate_file=T rnd_seed=666]]></command_line>
```

```
{'gamma_surface_vacancy': 750, 'slice_sample': 2000, 'surface': 180, 'vacancy': 420, 'dislocation_quadrupole': 100, 'gamma_surface':
6183, 'md_bulk': 60}
```

-		GAP_6
0	bcc_c12	199.05
1	bcc_c11	518.12
2	bcc_c44	143.12
3	surface_energy_100_unrelaxed	1.07

bulk_bcc







