

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>
```

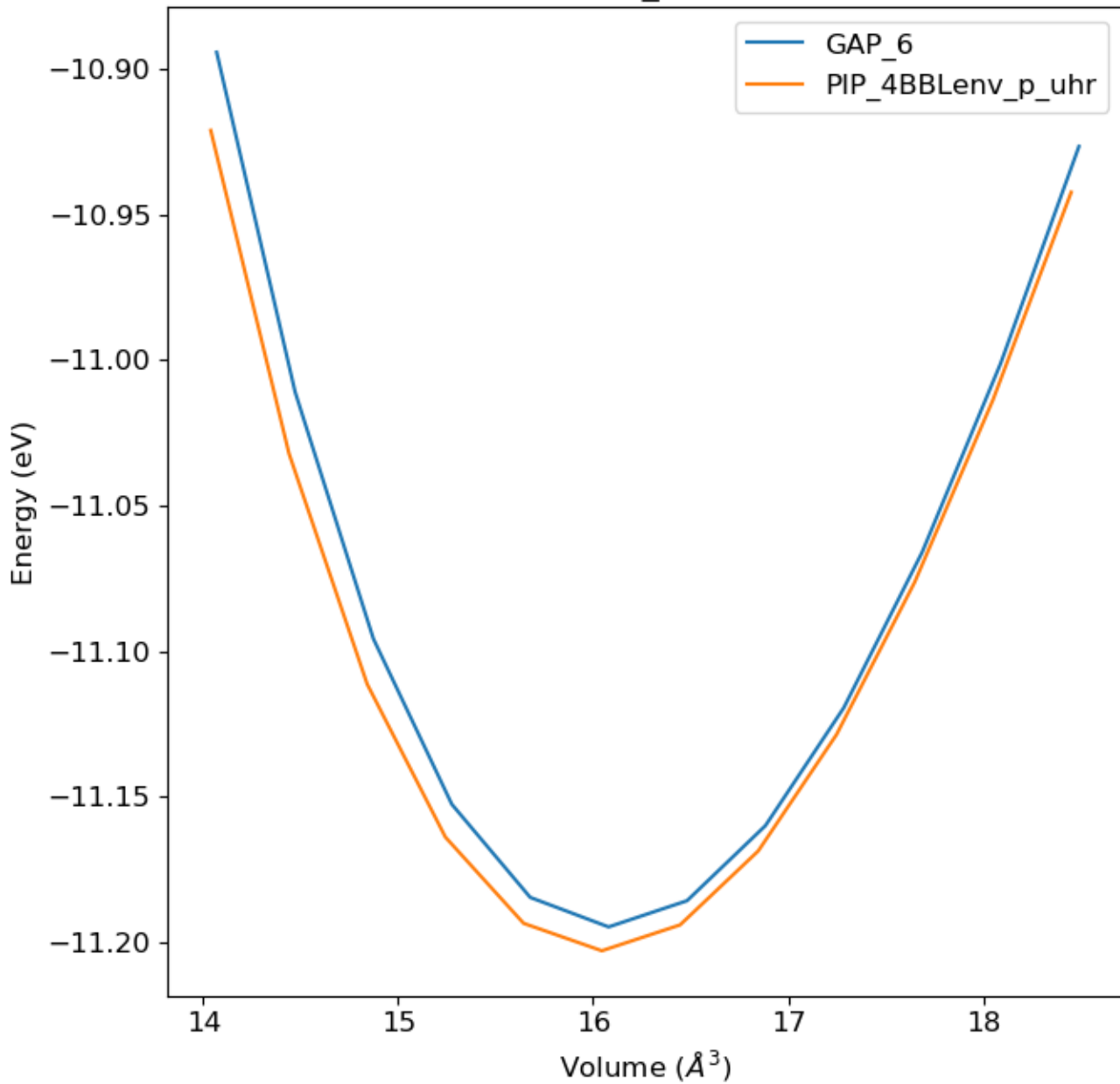
```
{'gamma_surface_vacancy': 1500, 'slice_sample': 4000, 'surface': 360, 'vacancy': 840, 'dislocation_quadrupole': 200, 'gamma_surface':
12366, 'md_bulk': 120}
```

PIP\_4BBLenv\_p\_uhr

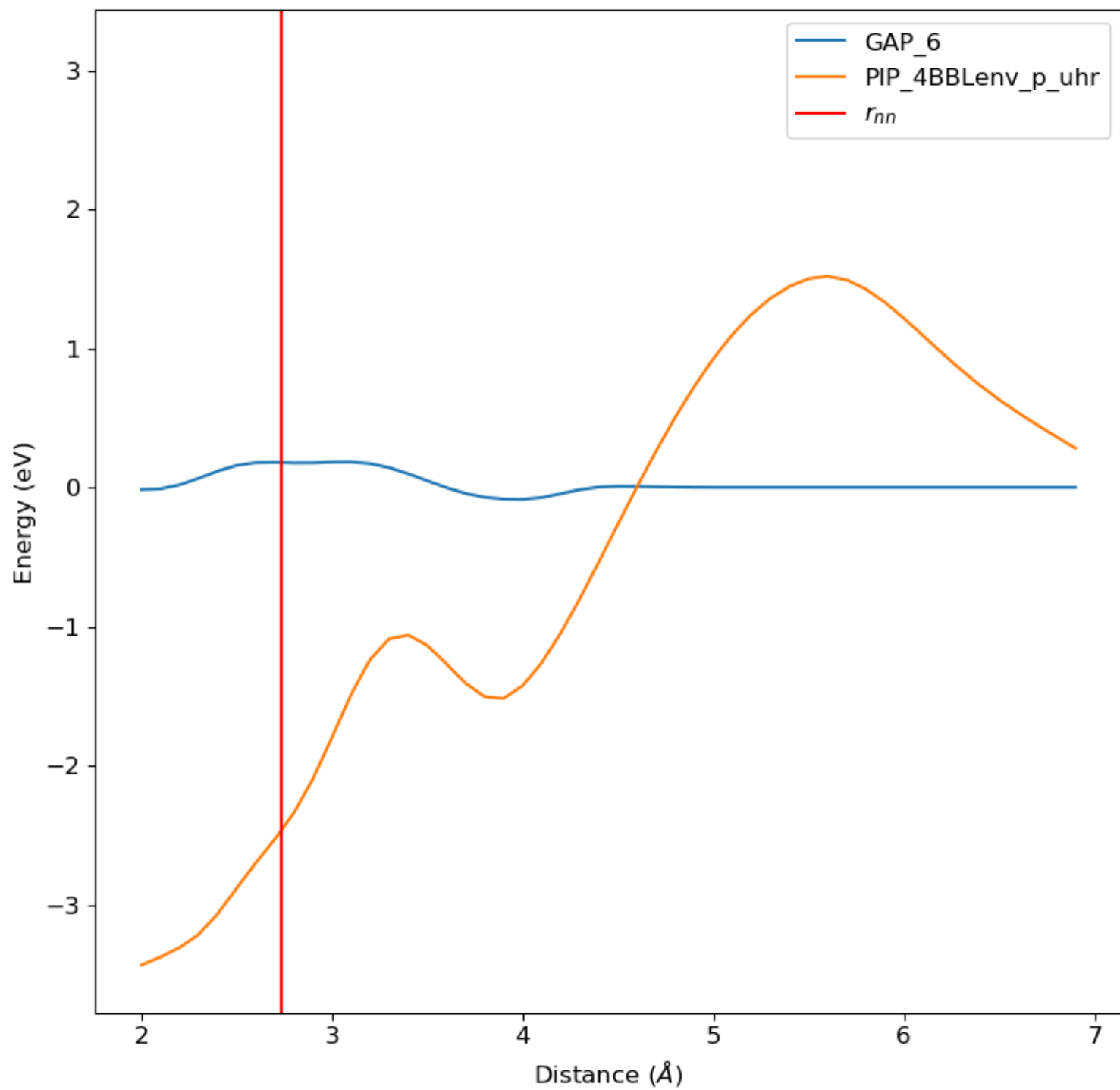
```
config_weights {gamma_surface_vacancy: [1.0, 0.5], dislocation_quadrupole: [1.0, 0.5], slice_sample: 1.0, surface: 1.0, vacancy: [1.0,
0.5], md_bulk: 1.0, gamma_surface: [1.0, 0.5]}
data_weights {F: 1.0, E: 10.0, V: 1.0}
num_configs {gamma_surface_vacancy: 750, dislocation_quadrupole: 100, slice_sample: 2000, surface: 180, vacancy: 420, md_bulk: 60,
gamma_surface: 6183}
db W_4BBLenv_med
```

| - |         | GAP_6  | PIP_4BBLe <sub>env</sub> -p_uhr |
|---|---------|--------|---------------------------------|
| 0 | bcc_c12 | 199.59 | -3%                             |
| 1 | bcc_c11 | 519.08 | -4%                             |
| 2 | bcc_c44 | 143.39 | 15%                             |

bulk\_bcc



## dimer



layer\_test

