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

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

PIP_4BBLenv_p_r

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

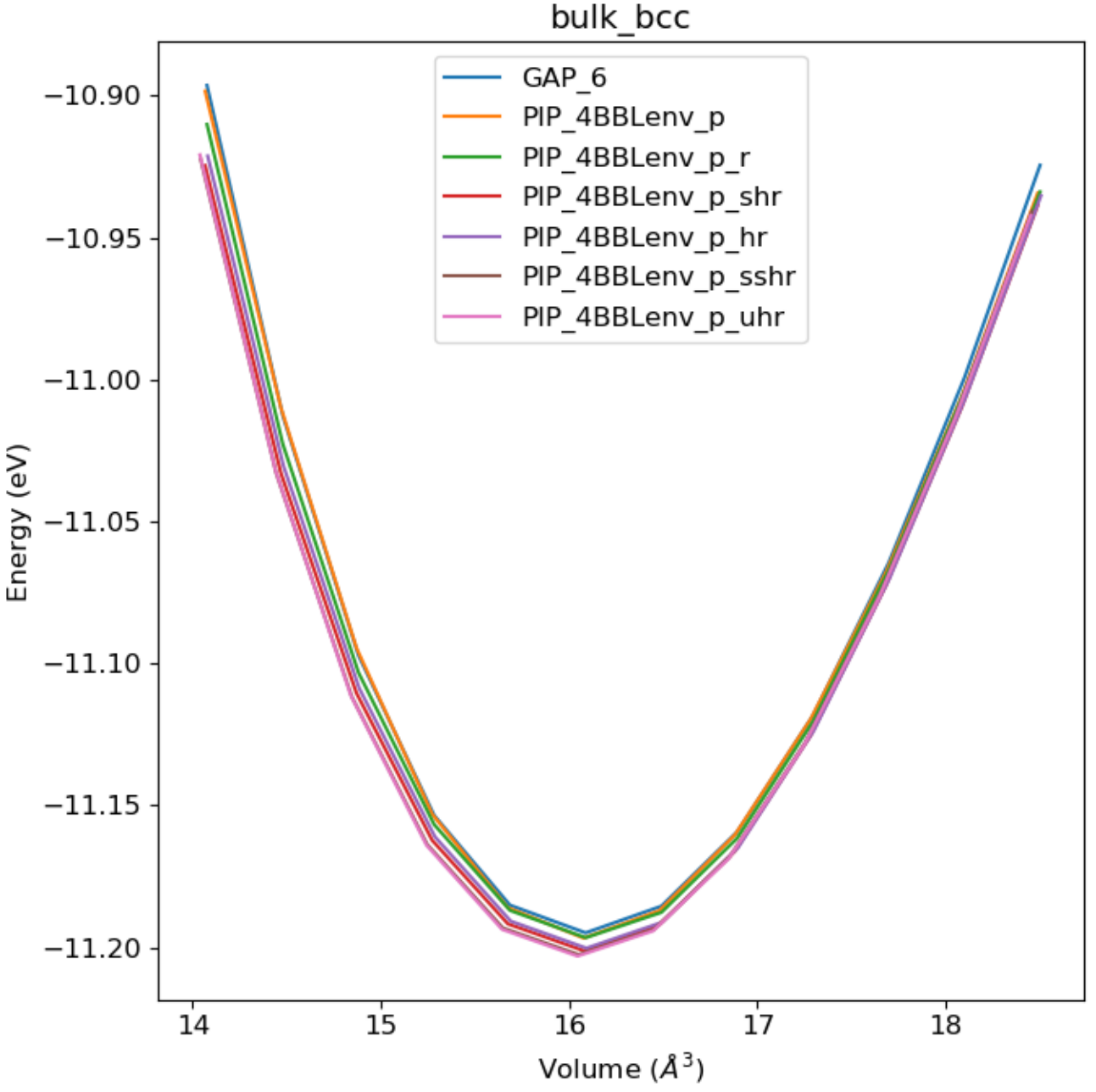
PIP_4BBLenv_p_shr

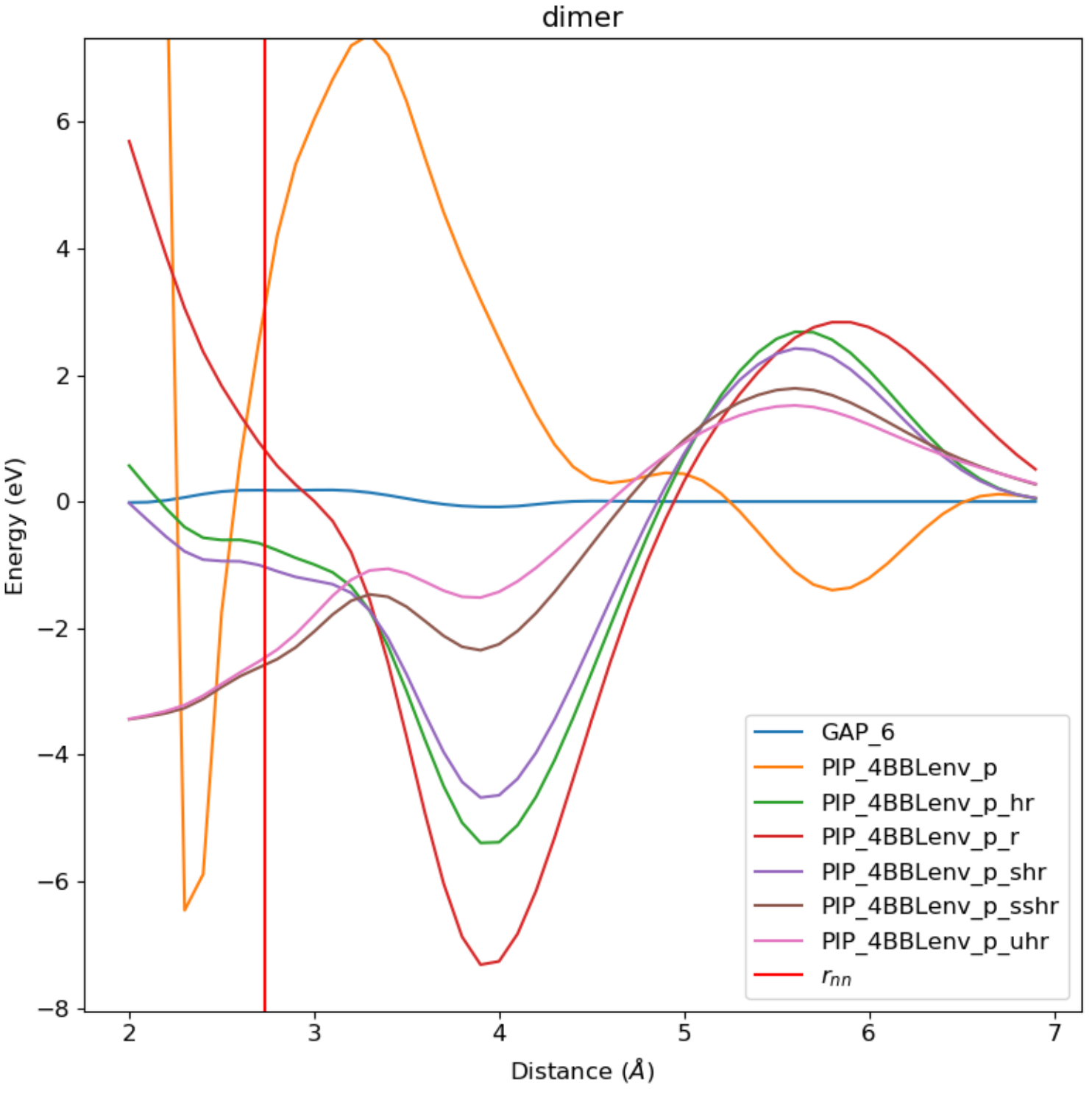
config_weights {gamma_surface_vacancy: [1.0, 0.5], dislocation_quadrupole: [1.0, 0.5], slice_sample: 1.0, surface: 1.0, vacancy: [1.0, 0.5], md_bulk: 1.0, gamma_surface: [1.0, 0.5]}
data_weights {F: 1.0, E: 10.0, V: 1.0}
num_configs {gamma_surface_vacancy: 750, dislocation_quadrupole: 100, slice_sample: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

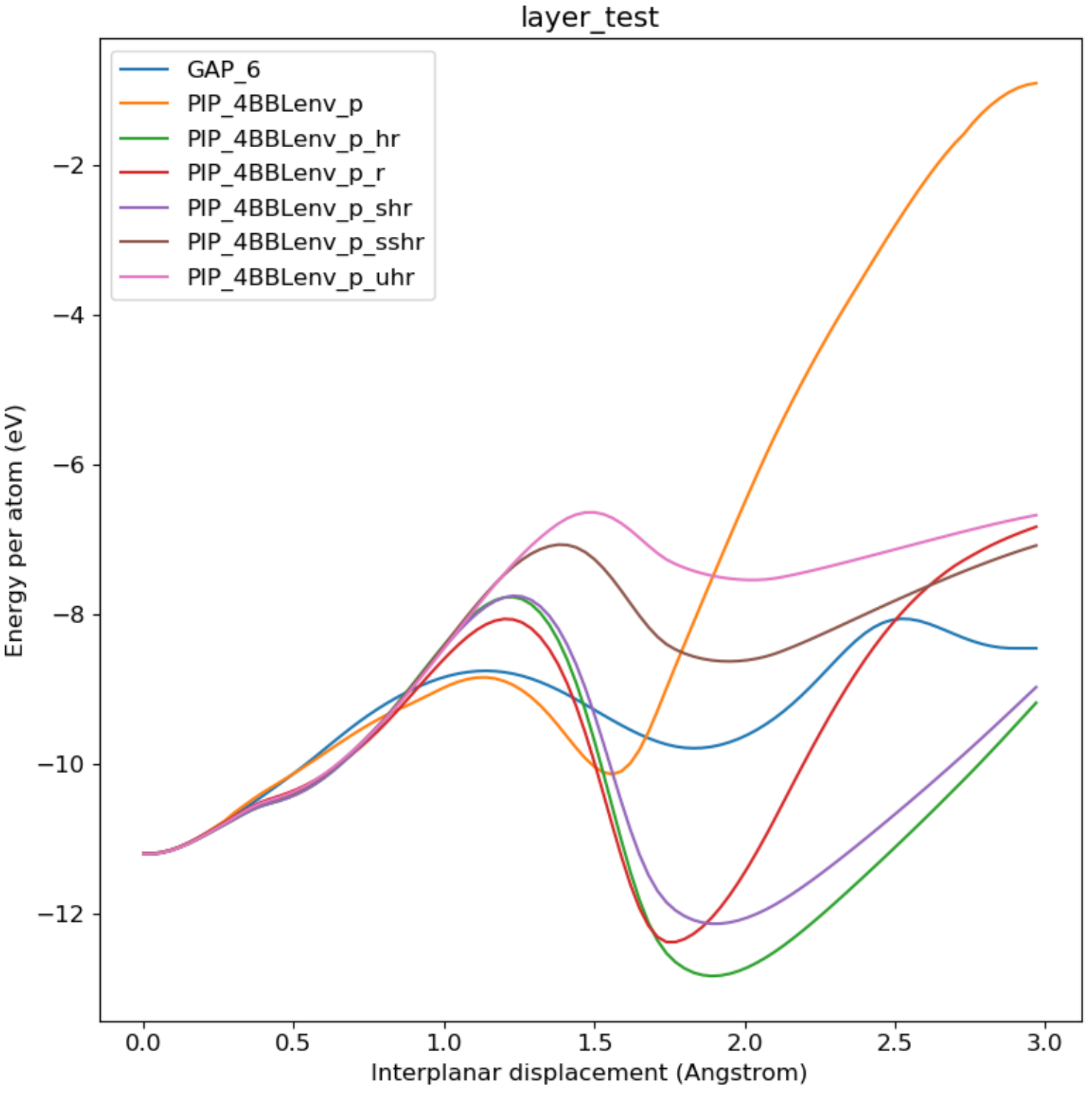
PIP_4BBLenv_p_hr

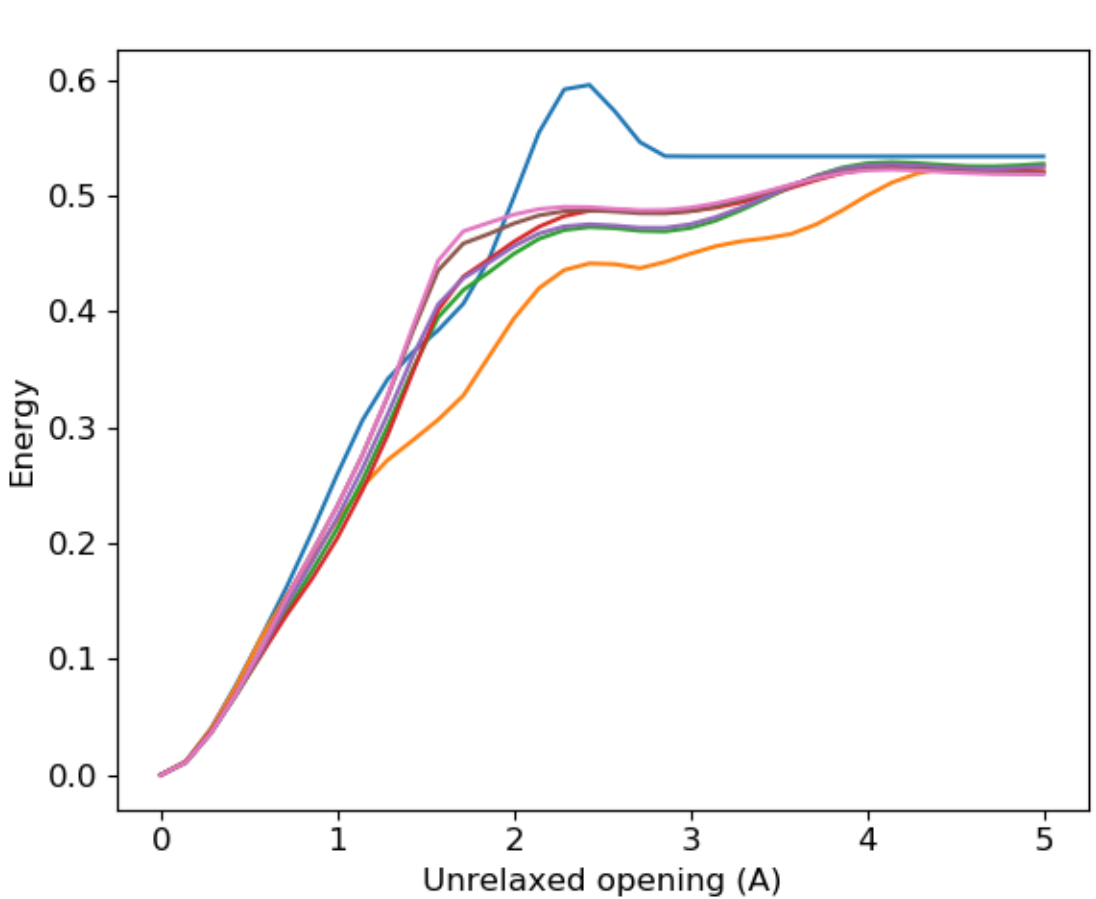
config_weights {gamma_surface_vacancy: [1.0, 0.5], dislocation_quadrupole: [1.0, 0.5], slice_sample: 1.0, surface: 1.0, vacancy: [1.0, 0.5], md_bulk: 1.0, gamma_surface: [1.0, 0.5]}
data_weights {F: 1.0, E: 10.0, V: 1.0}
num_configs {gamma_surface_vacancy: 750, dislocation_quadrupole: 100, slice_sample: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

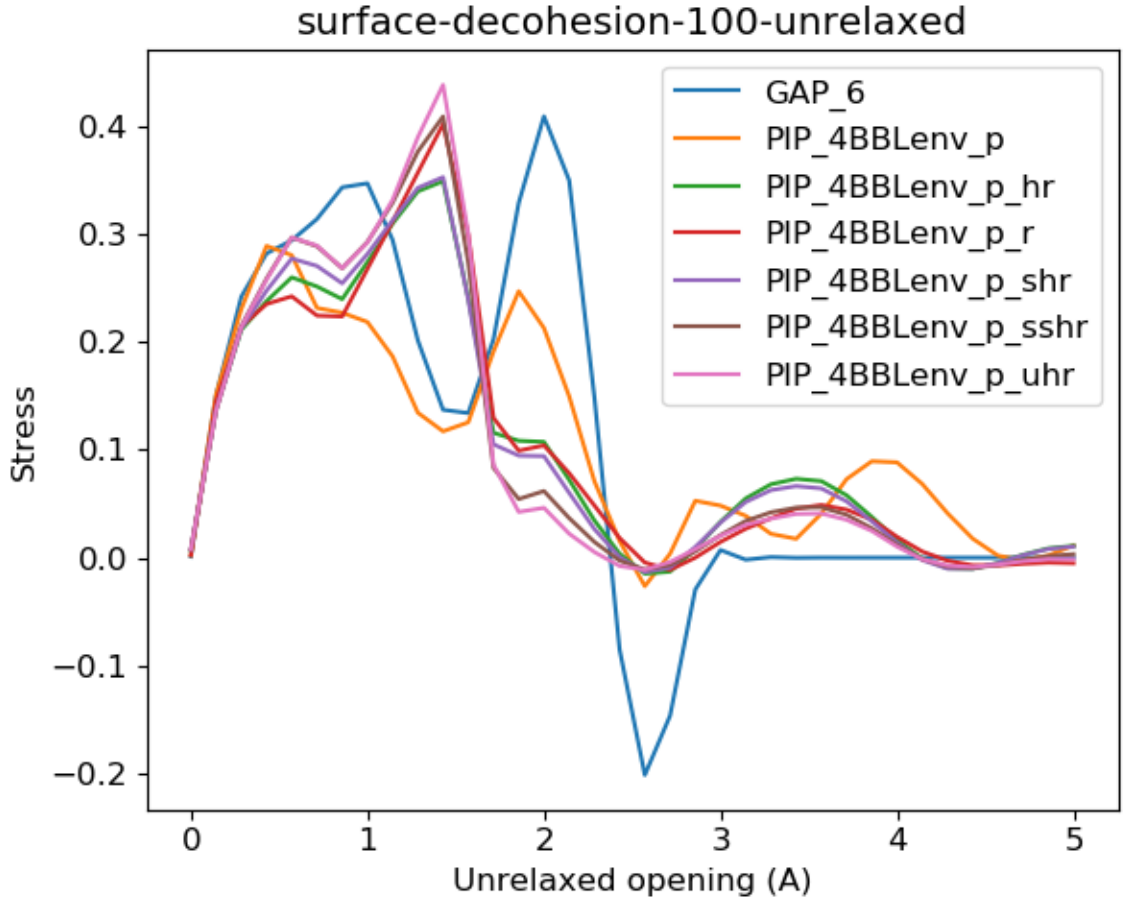
	-	GAP_6	PIP_4BBLenv_p	PIP_4BBLenv_p_hr	PIP_4BBLenv_p_r	PIP_4BBLenv_p_shr	PIP_4BBLenv_p_sshr
0	bcc_c12	199.05	6%	0%	0%	0%	-3%
1	bcc_c11	518.12	2%	-5%	-4%	-5%	-5%
2	bcc_c44	143.12	4%	6%	1%	8%	13%

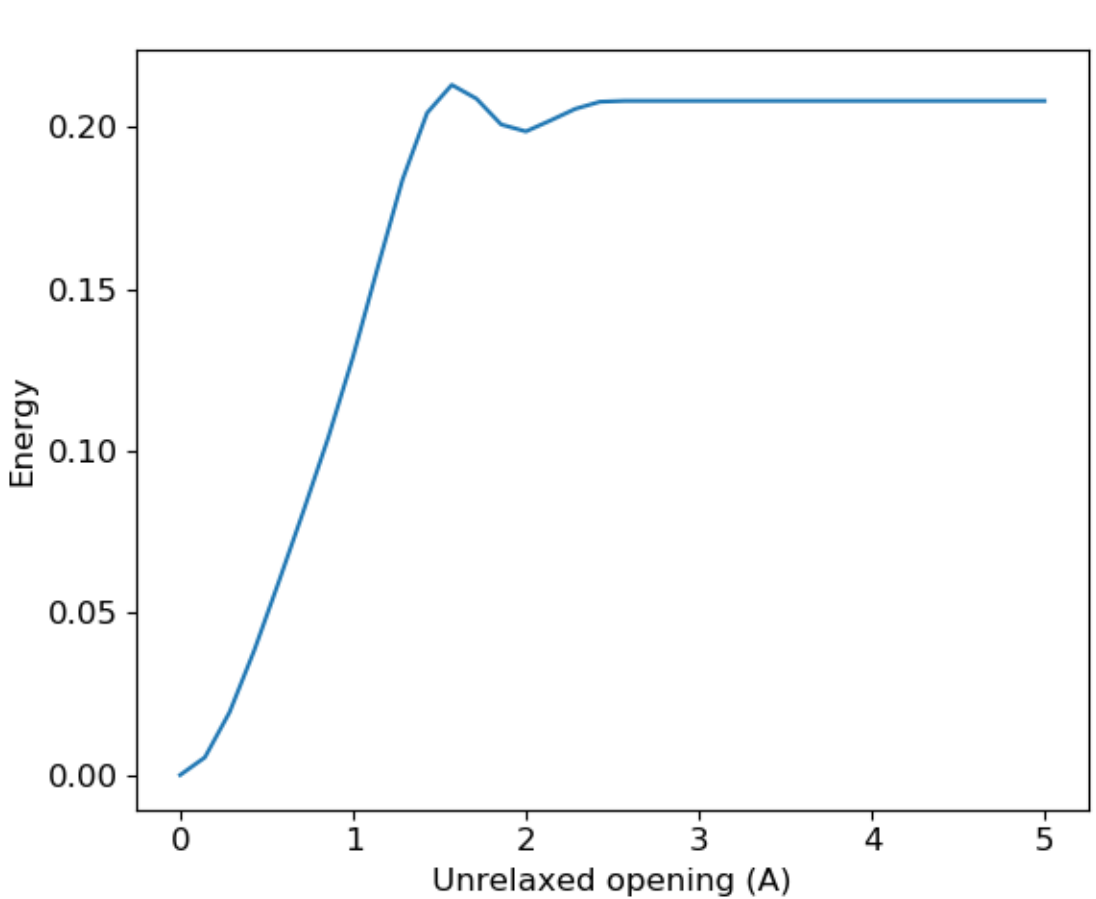

bulk_bcc
GAP_6
PIP_4BBLenv_p
PIP_4BBLenv_p_r
PIP_4BBLenv_p_shr
PIP_4BBLenv_p_hr
PIP_4BBLenv_p_sshr
PIP_4BBLenv_p_uhr
−10.90
−10.95
−11.00
−11.05
−11.10
−11.15
−11.20
Energy (eV)
14
15
16
17
18
Volume ($Å^3$)

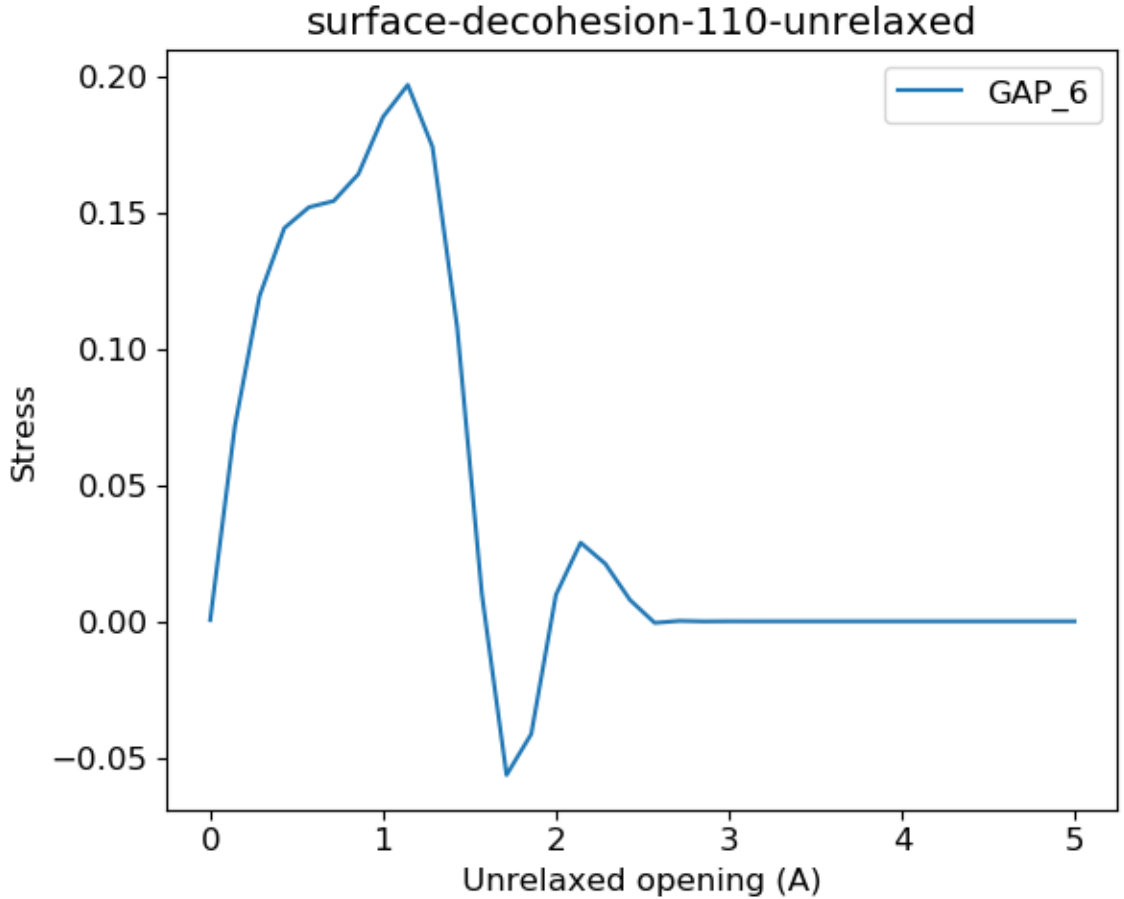

dimer
Energy (eV)
Distance (Å)
6
4
2
0
−2
−4
−6
−8
2
3
4
5
6
7
GAP_6
PIP_4BBLenv_p
PIP_4BBLenv_p_hr
PIP_4BBLenv_p_r
PIP_4BBLenv_p_shr
PIP_4BBLenv_p_sshr
PIP_4BBLenv_p_uhr
r_{nn}

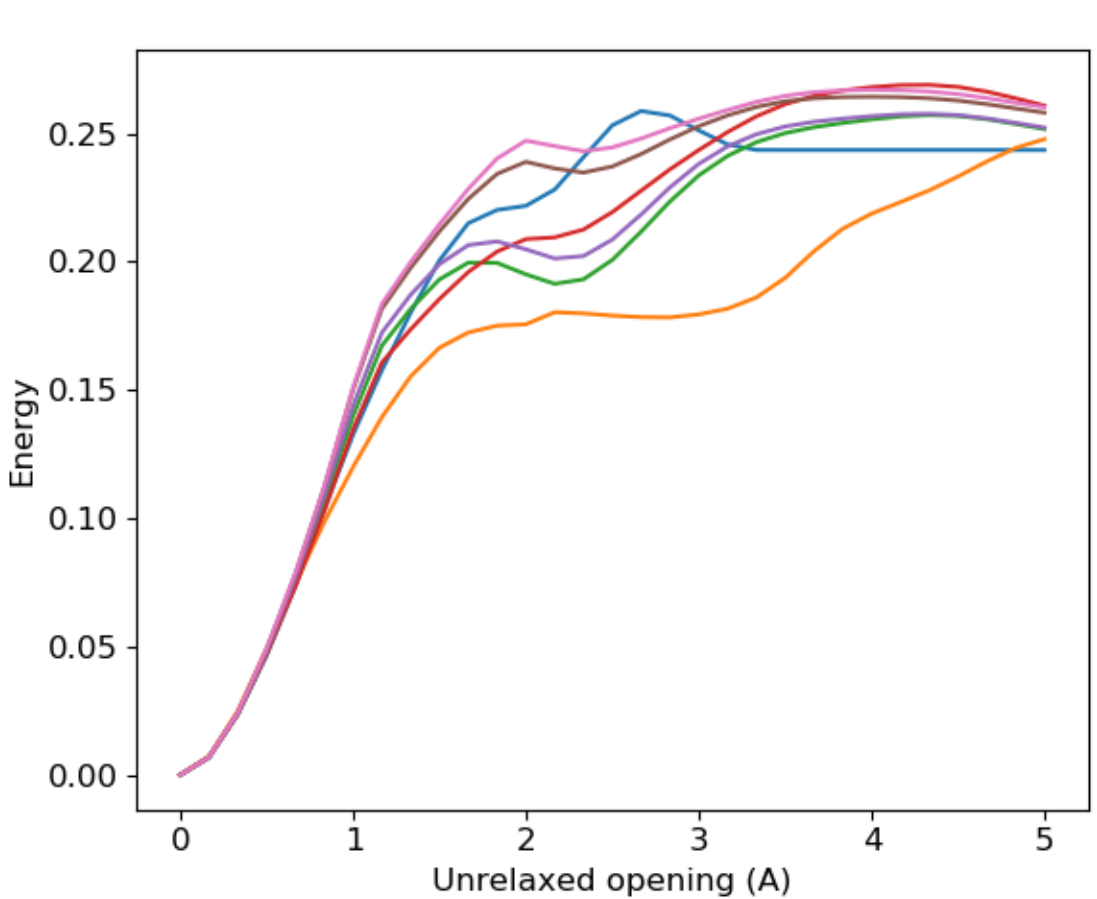

layer_test
GAP_6
PIP_4BBLenv_p
PIP_4BBLenv_p_hr
PIP_4BBLenv_p_r
PIP_4BBLenv_p_shr
PIP_4BBLenv_p_sshr
PIP_4BBLenv_p_uhr
−2
−4
−6
−8
−10
−12
Energy per atom (eV)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Interplanar displacement (Angstrom)

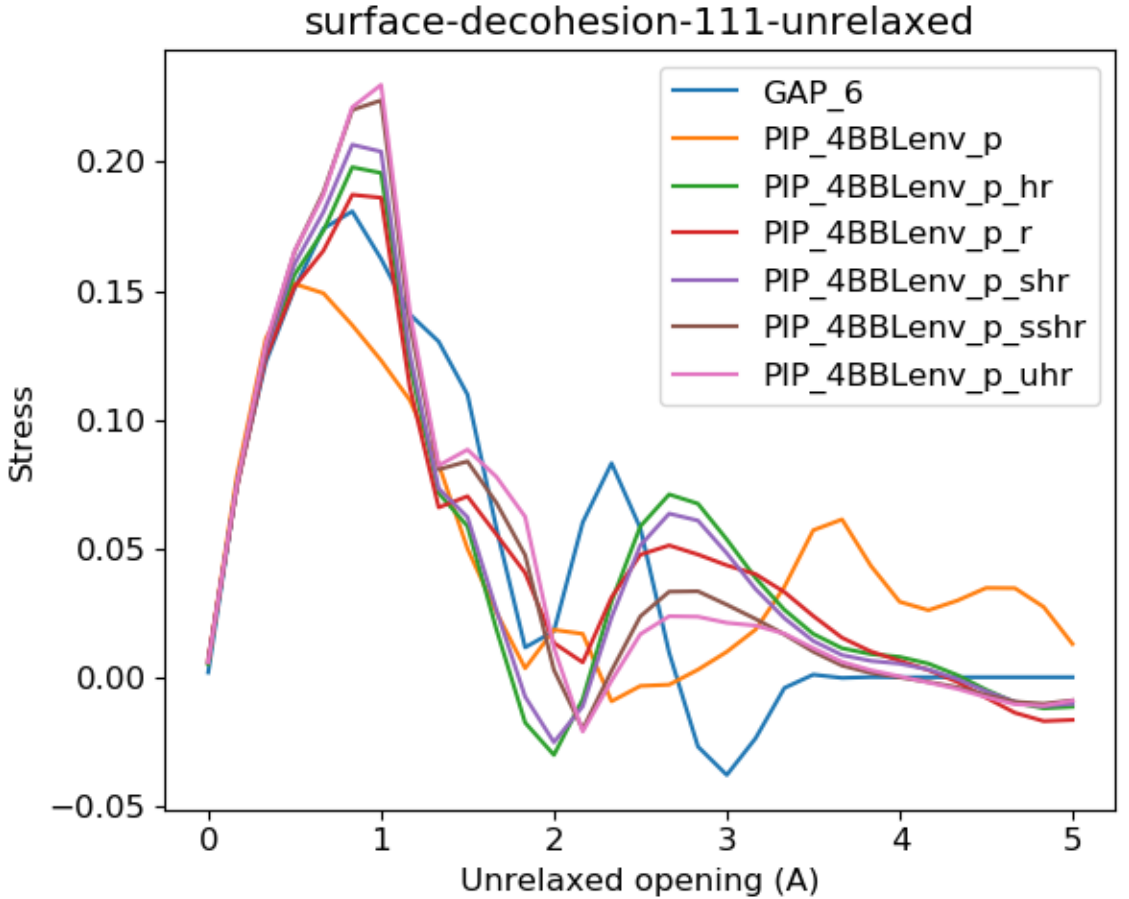

Energy
Unrelaxed opening (A)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0
1
2
3
4
5


surface-decohesion-100-unrelaxed
Stress
Unrelaxed opening (A)
GAP_6
PIP_4BBLenv_p
PIP_4BBLenv_p_hr
PIP_4BBLenv_p_r
PIP_4BBLenv_p_shr
PIP_4BBLenv_p_sshr
PIP_4BBLenv_p_uhr
−0.2
−0.1
0.0
0.1
0.2
0.3
0.4
0
1
2
3
4
5


Energy
0.20
0.15
0.10
0.05
0.00
0
1
2
3
4
5
Unrelaxed opening (A)


surface-decohesion-110-unrelaxed
GAP_6
Stress
0.20
0.15
0.10
0.05
0.00
−0.05
0
1
2
3
4
5
Unrelaxed opening (A)


Energy
0.25
0.20
0.15
0.10
0.05
0.00
0
1
2
3
4
5
Unrelaxed opening (A)


surface-decohesion-111-unrelaxed
Stress
0.20
0.15
0.10
0.05
0.00
−0.05
0
1
2
3
4
5
Unrelaxed opening (A)
GAP_6
PIP_4BBLenv_p
PIP_4BBLenv_p_hr
PIP_4BBLenv_p_r
PIP_4BBLenv_p_shr
PIP_4BBLenv_p_sshr
PIP_4BBLenv_p_uhr