

GAP

```
<command_line><![CDATA[ at_file=si_iter6_database.xyz gap={soap l_max=12 n_max=10 atom_sigma=0.5 zeta=4 cutoff=5.0
cutoff_transition_width=1.0 central_weight=1.0 n_sparse=9000 delta=3.0 f0=0.0 covariance_type=dot_product
sparse_method=cur_points} default_sigma={0.001 0.1 0.05 0.0}
config_type_sigma={liq:0.003:0.15:0.2:0.0:amorph:0.01:0.2:0.4:0.0:sp:0.01:0.2:0.4:0.0} energy_parameter_name=dft_energy
force_parameter_name=dft_force virial_parameter_name=dft_virial config_type_parameter_name=config_type sparse_jitter=1.0e-8
e0_offset=2.0 core_param_file=glue.xml core_ip_args={IP Glue} gp_file=gp_iter6_sparse9k.xml]]></command_line>
```

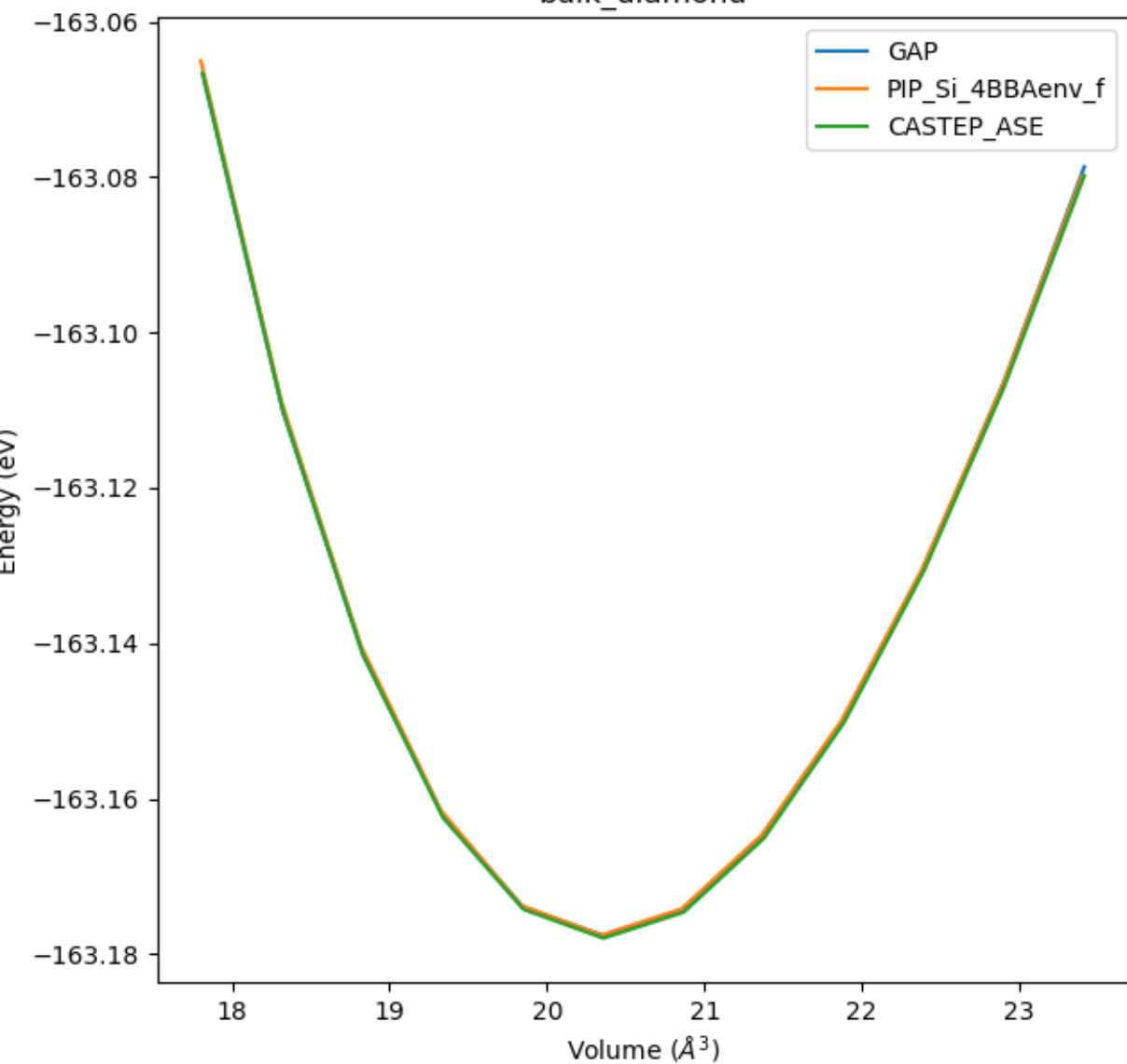
```
{'bt': 445, 'hcp': 49, 'crack_110_1-10': 7, 'surface_111': 28, 'surface_110': 26, 'sp2': 51, 'sp': 100, 'crack_111_1-10': 10, 'dia': 489,
'isolated_atom': 1, 'bcc': 49, 'vacancy': 100, '111adatom': 11, 'sh': 223, 'bc8': 49, 'liq': 76, 'surface_001': 29, 'hex_diamond': 49, 'st12': 49,
'amorph': 31, 'fcc': 49}
```

PIP_Si_4BBAenv_f

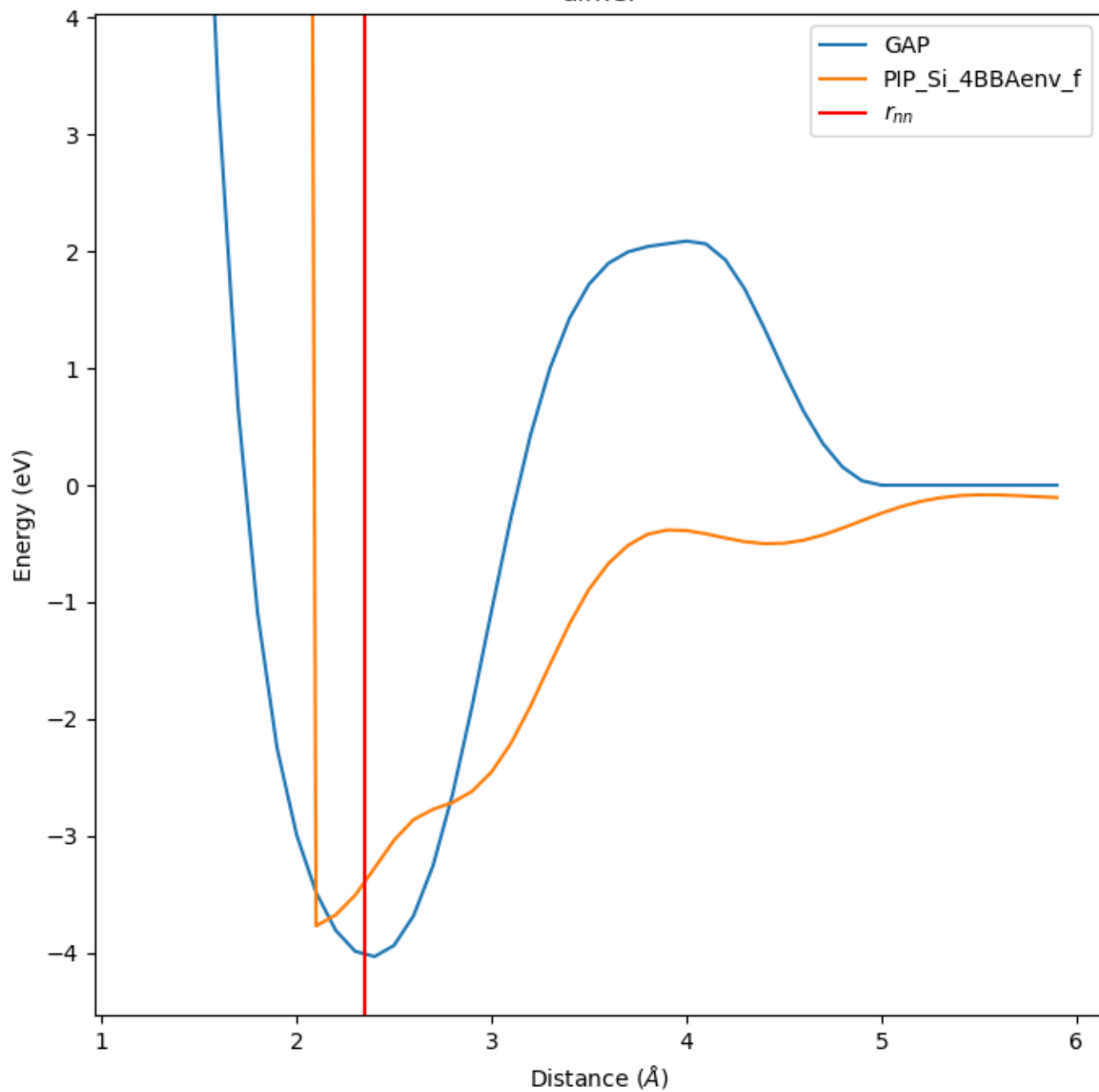
```
config_weights {surface_111: 1.0, surface_110: 1.0, sp2: 5.0, dia: 10.0, surface_001: 1.0}
data_weights {F: 1.0, E: 10.0, V: 1.0}
num_configs {divacancy: 78, vacancy: 211, screw_disloc: 19, st12: 49, hcp: 49, interstitial: 115, hex_diamond: 49, 111adatom: 11,
decohesion: 33, bc8: 49, liq: 76, surface_001: 29, sp2: 51, bt: 445, fcc: 49, surface_111_3x3_das: 1, crack_111_1: 10, crack_110_1: 7,
surface_111: 47, surface_110: 26, sp: 100, dia: 489, bcc: 49, sh: 223, surface_111_pandey: 50, amorph: 159}
db Si_4B_BAenv_med.jld2
```

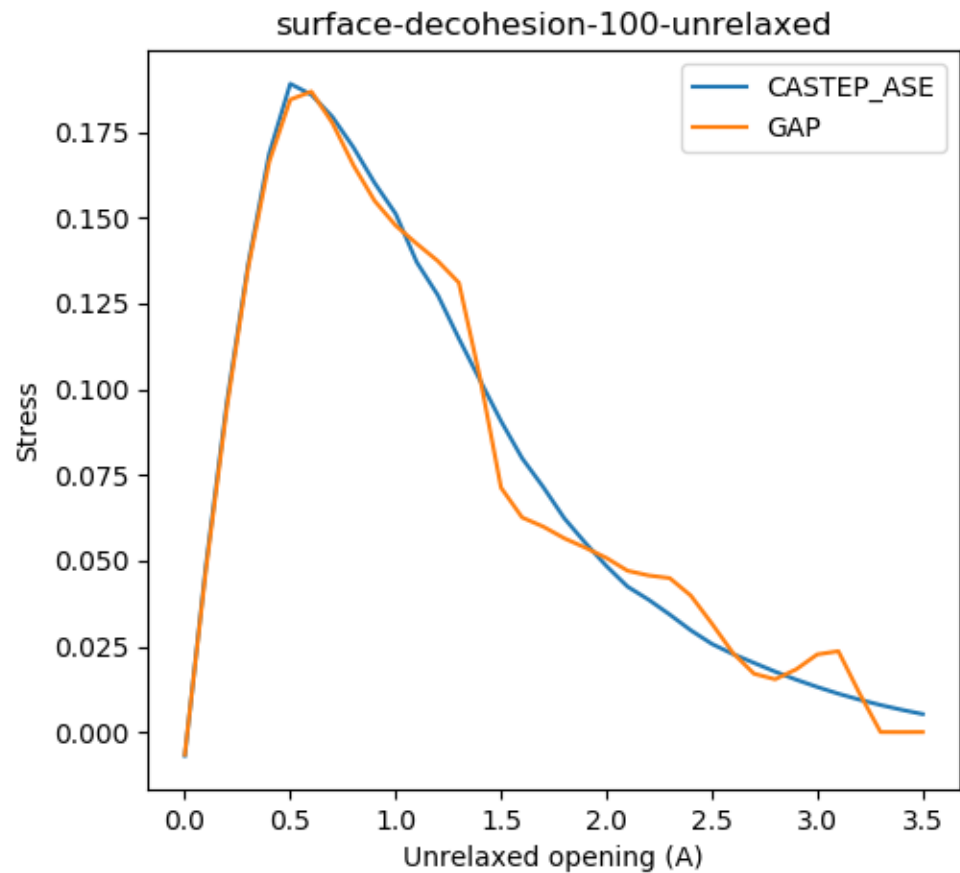
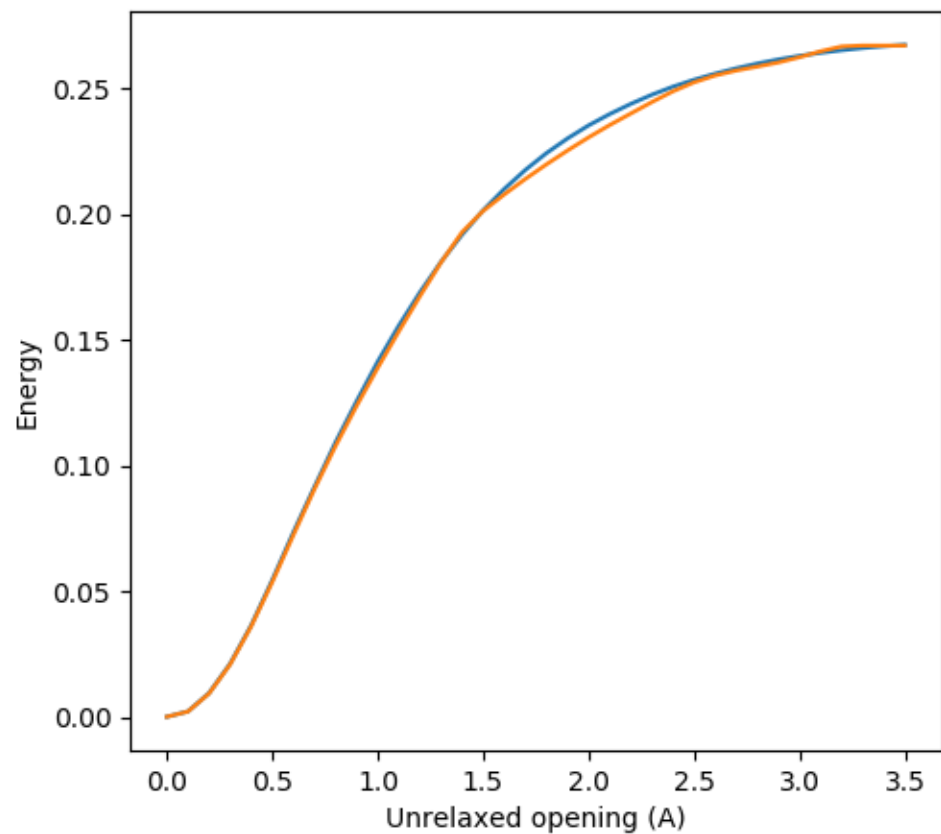
-		CASTEP_ASE	GAP	PIP_Si_4BBAenv_f
0	diamond_bulk_modulus	88.60	0%	1%
1	diamond_c12	56.25	3%	6%
2	diamond_c11	153.29	-2%	-2%
3	diamond_c44	72.18	-7%	-4%
4	diamond_a0	5.46	0%	0%

bulk_diamond



dimer





111_layer_test

