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}

GAP_4

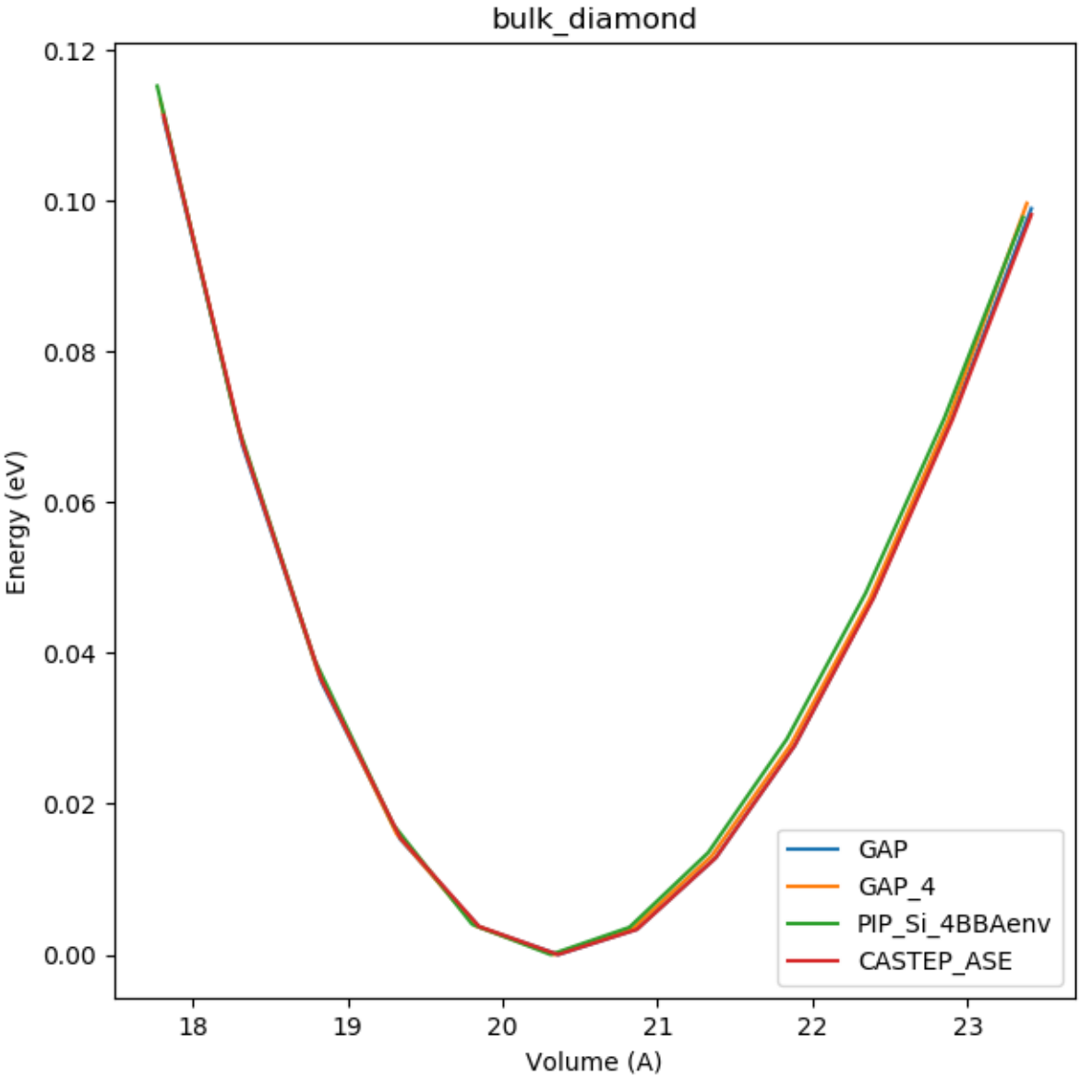
<command_line><![CDATA[at_file=data_all.xyz descriptor_str={soap l_max=12 n_max=10 atom_sigma=0.5 zeta=4 cutoff=5.0 cutoff_transition_width=1.0 n_sparseX=8500 delta=1.0 f0=0.0 covariance_type=dot_product sparse_method=kmeans} default_sigma={0.003 0.25 0.2} energy_parameter_name=DFT_energy force_parameter_name=DFT_force virial_parameter_name=DFT_virial sparse_jitter=1.0e-8 e0_offset=2.0 core_param_file=ip.parms.Glue.4.xml ip_args={IP Glue} gp_file=gp_soap_all_12_10_0.5_4_5.0_8500.xml]]></command_line>

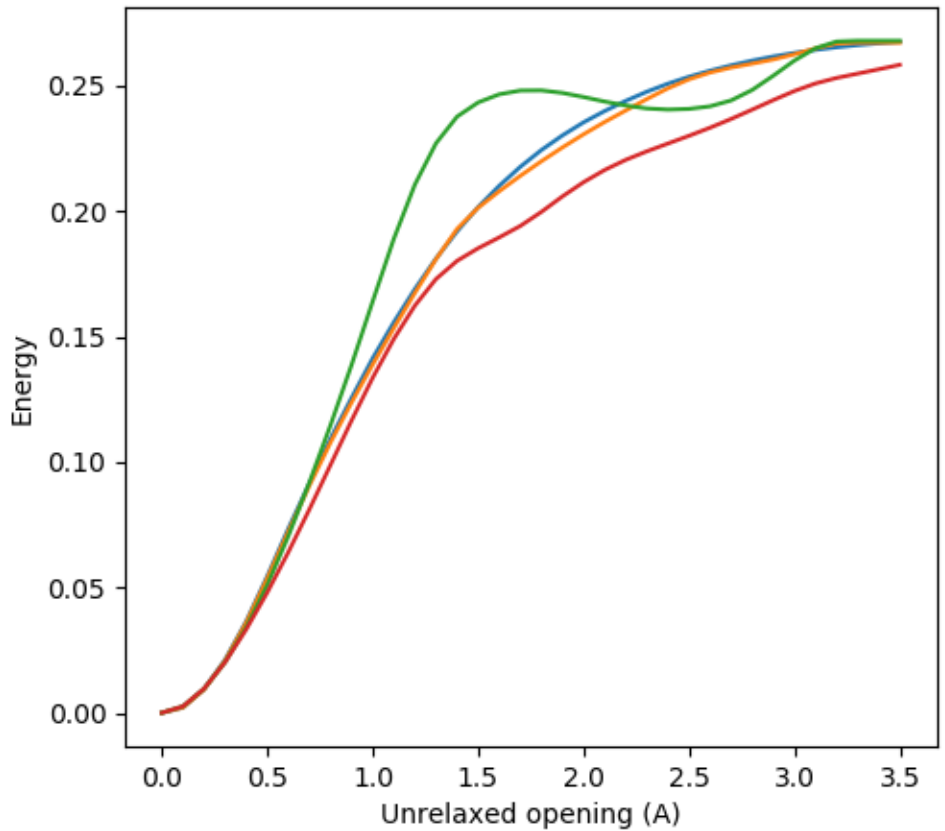
{'md': 5289, 'liquid': 2, 'crack_110_1-10': 7, 'min': 1161, 'crack_111_1-10': 10, 'dia': 489, 'isolated_atom': 1, 'surface_001_z': 10, 'bt': 445, 'sh': 163, 'liq': 74, 'surface_111_y': 28, 'amorph': 31, 'surface_110_z': 12}

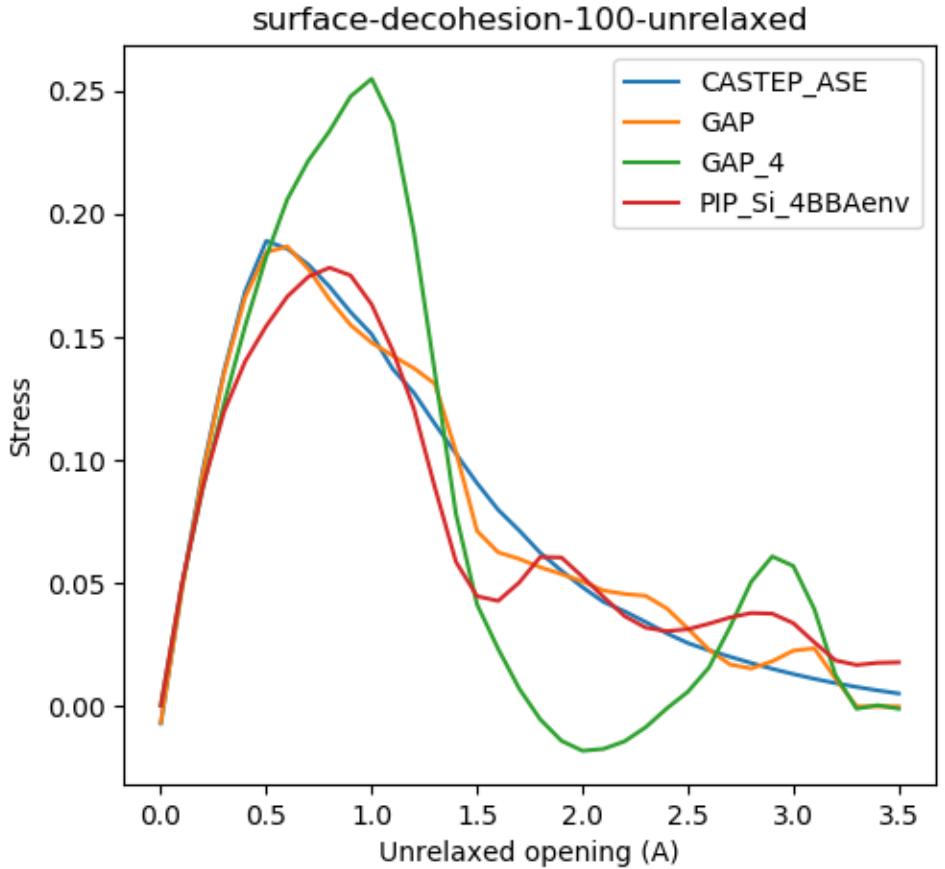
PIP_Si_4BBAenv

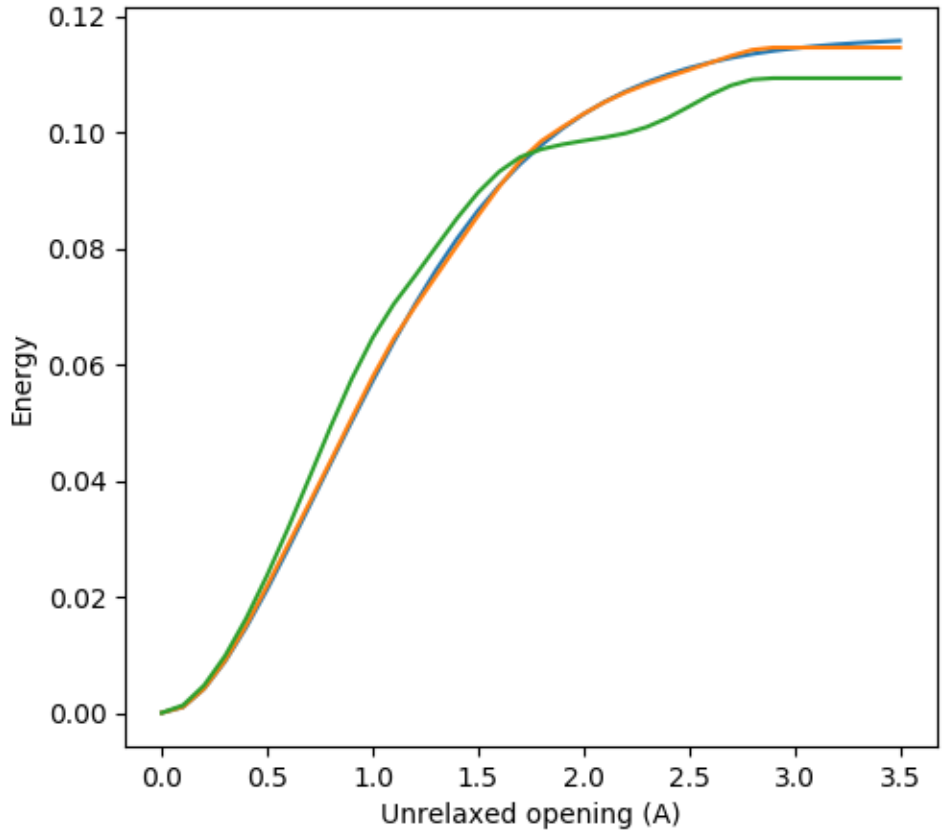
config_weights {surface_111: 1.0, surface_110: 1.0, dia: 1.0, surface_001: 1.0}
data_weights {F: 1.0, E: 100.0, V: 1.0}
num_configs {divacancy: 78, vacancy: 211, screw_disloc: 19, st12: 49, hcp: 49, interstitial: 115, hex_diamond: 49, 111adatom: 11, decohesion: 33, bc8: 49, liq: 76, surface_001: 29, 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

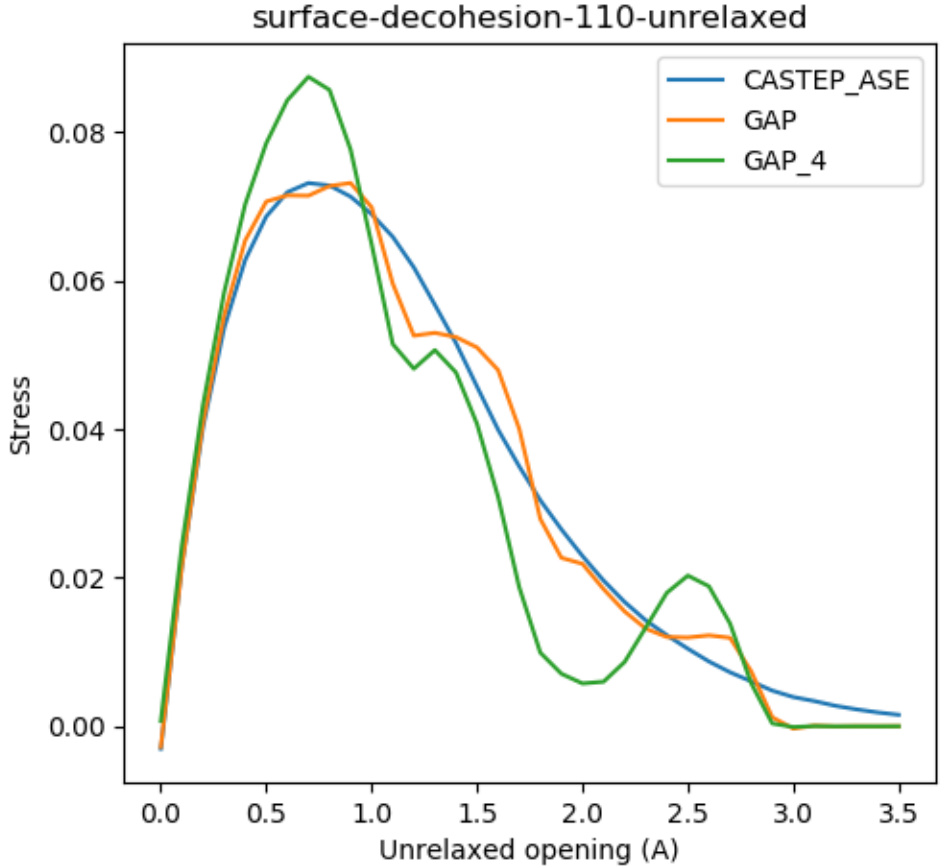
	-	CASTEP_ASE	GAP	GAP_4	PIP_Si_4BBAenv
0	diamond_bulk_modulus	88.60	0%	0%	8%
1	diamond_c12	56.25	3%	-5%	16%
2	diamond_c11	153.29	-2%	5%	1%
3	diamond_c44	72.18	-7%	-1%	-2%
4	diamond_a0	5.46	0%	0%	0%
5	surface_energy_100_unrelaxed	0.27	0%	0%	0%
6	surface_energy_111_unrelaxed	0.10	-3%	-8%	-11%

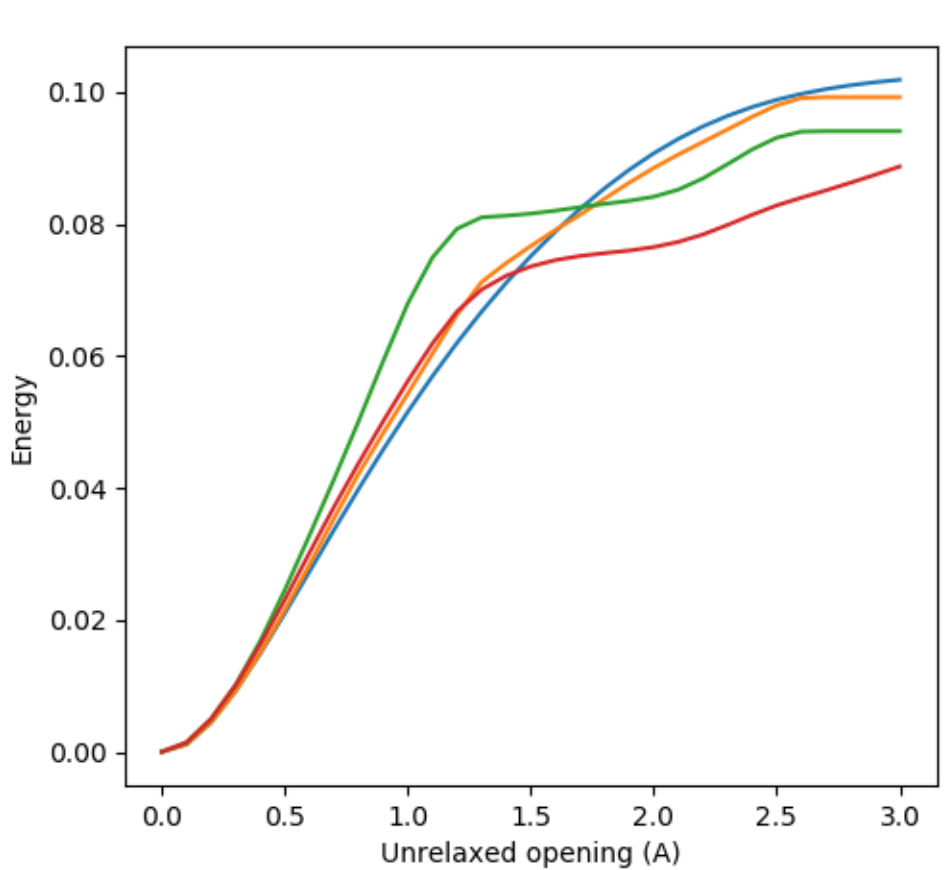

bulk_diamond
0.12
0.10
0.08
0.06
0.04
0.02
0.00
Energy (eV)
18
19
20
21
22
23
Volume (A)
GAP
GAP_4
PIP_Si_4BBAenv
CASTEP_ASE

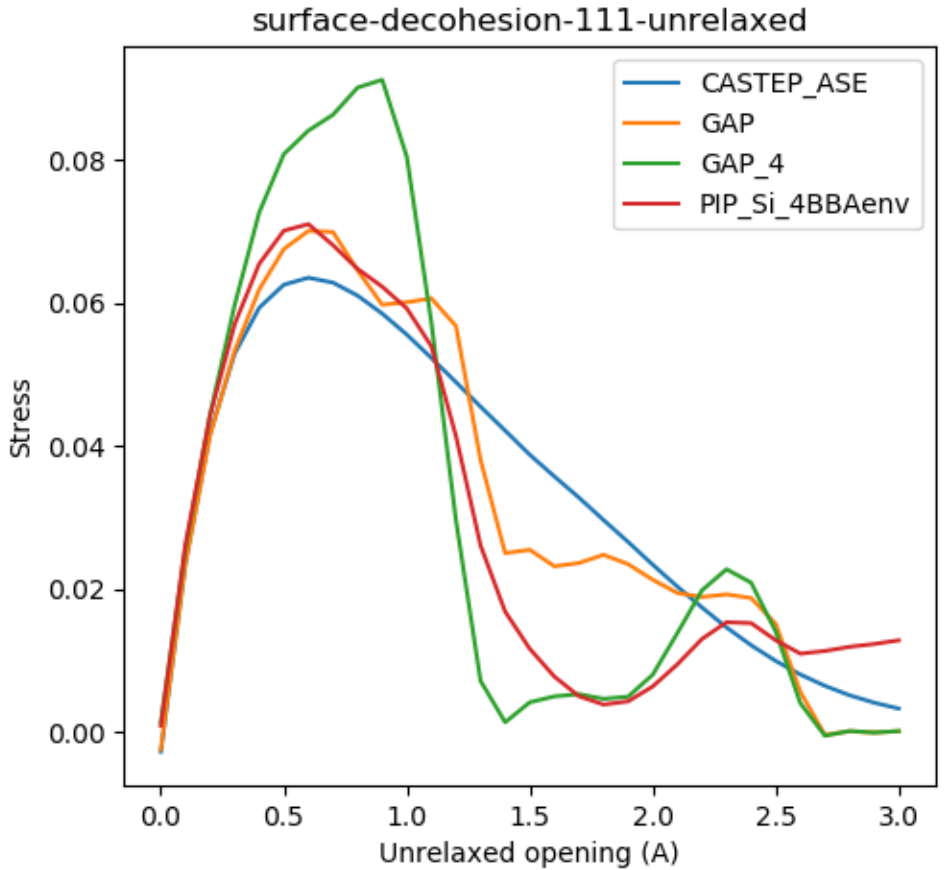

Energy
0.00
0.05
0.10
0.15
0.20
0.25
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Unrelaxed opening (A)

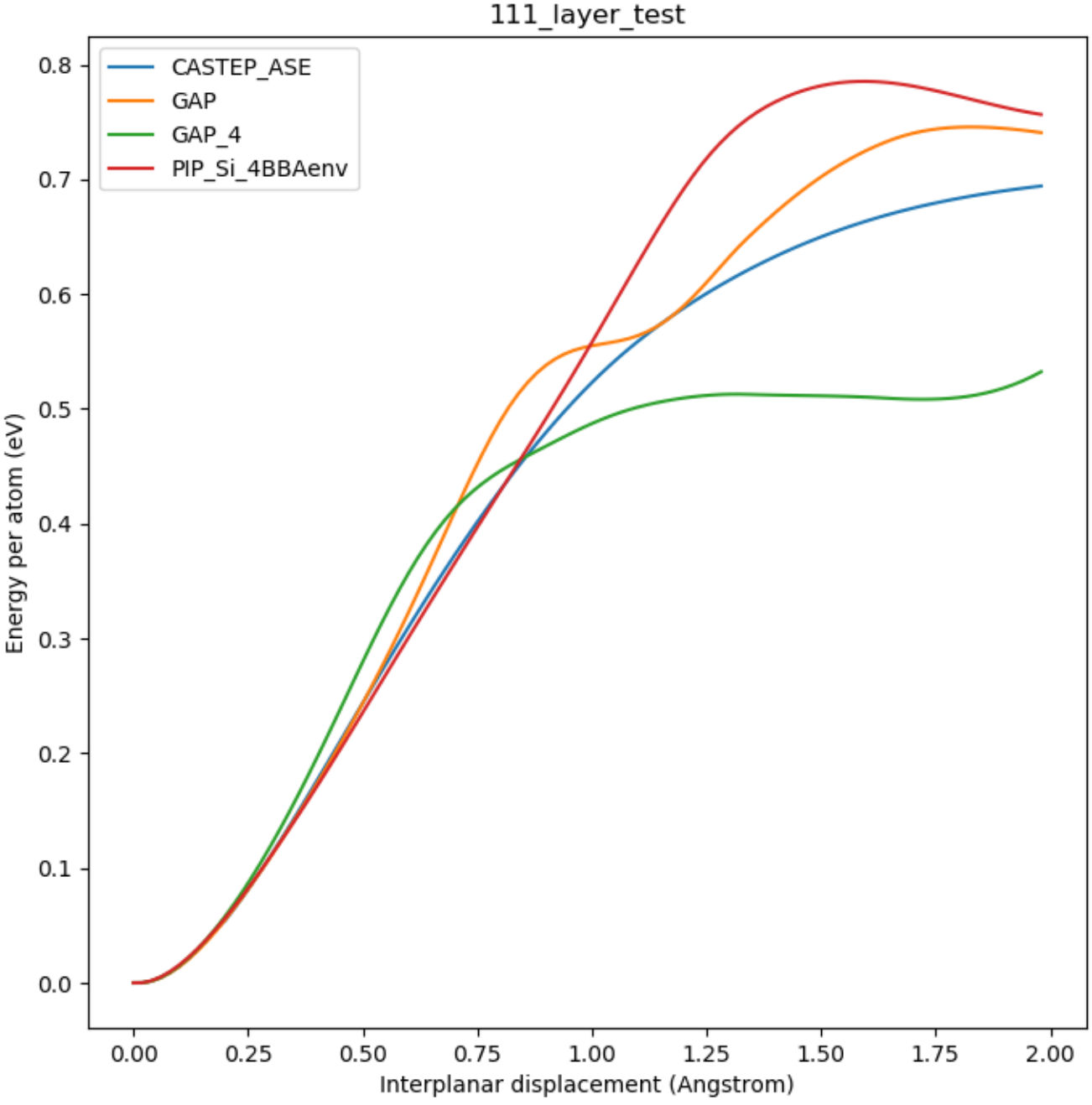

surface-decohesion-100-unrelaxed
CASTEP_ASE
GAP
GAP_4
PIP_Si_4BBAenv
Stress
0.00
0.05
0.10
0.15
0.20
0.25
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Unrelaxed opening (A)


0.12
0.10
0.08
0.06
0.04
0.02
0.00
Energy
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Unrelaxed opening (A)


surface-decohesion-110-unrelaxed
CASTEP_ASE
GAP
GAP_4
0.08
0.06
0.04
0.02
0.00
Stress
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Unrelaxed opening (A)


0.10
0.08
0.06
0.04
0.02
0.00
Energy
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Unrelaxed opening (A)


surface-decohesion-111-unrelaxed
CASTEP_ASE
GAP
GAP_4
PIP_Si_4BBAenv
0.08
0.06
0.04
0.02
0.00
Stress
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Unrelaxed opening (A)


111_layer_test
CASTEP_ASE
GAP
GAP_4
PIP_Si_4BBAenv
Energy per atom (eV)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
Interplanar displacement (Angstrom)