GAP_hcp_bcc_varcell

<command_line><![CDATA[at_file=hcp_bcc_varcell_k8.xyz gap="distance_Nb order=2 cutoff=9.0 covariance_type=ard_se n_sparse=20 theta_uniform=1.0 delta=0.003 compact_clusters=T :soap cutoff=4.0 covariance_type=dot_product n_sparse=2000 delta=0.095 sparse_method=cur_points l_max=10 n_max=10 zeta=4 atom_sigma=0.5" e0=-4.42384810052 sparse_separate_file=F gp_file=gp_soap_hcp_bcc_varcell.xml default_sigma={0.005 0.5 0.5 0.0}]]></command_line>
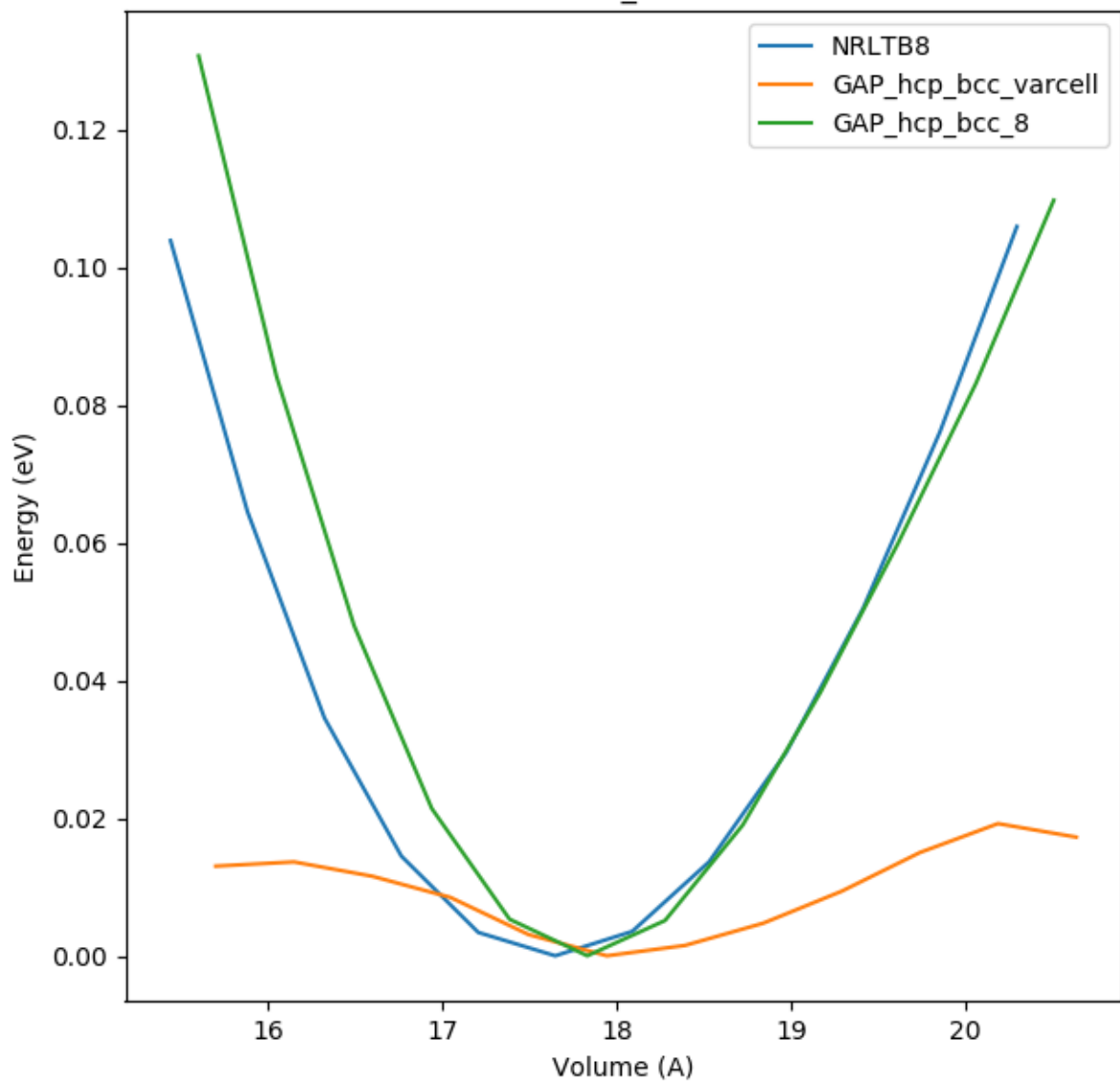
{}

GAP_hcp_bcc_8

<command_line><![CDATA[at_file=hcp_to_bcc_24_8.xyz gap="distance_Nb order=2 cutoff=9.0 covariance_type=ard_se n_sparse=20 theta_uniform=1.0 delta=0.003 compact_clusters=T :soap cutoff=4.0 covariance_type=dot_product n_sparse=2000 delta=0.095 sparse_method=cur_points l_max=10 n_max=10 zeta=4 atom_sigma=0.5" e0=-4.334618118602442 sparse_separate_file=F gp_file=gp_soap_hcp_bcc_24_8.xml default_sigma={0.000001 0.05 0.5 0.0}]]></command_line>
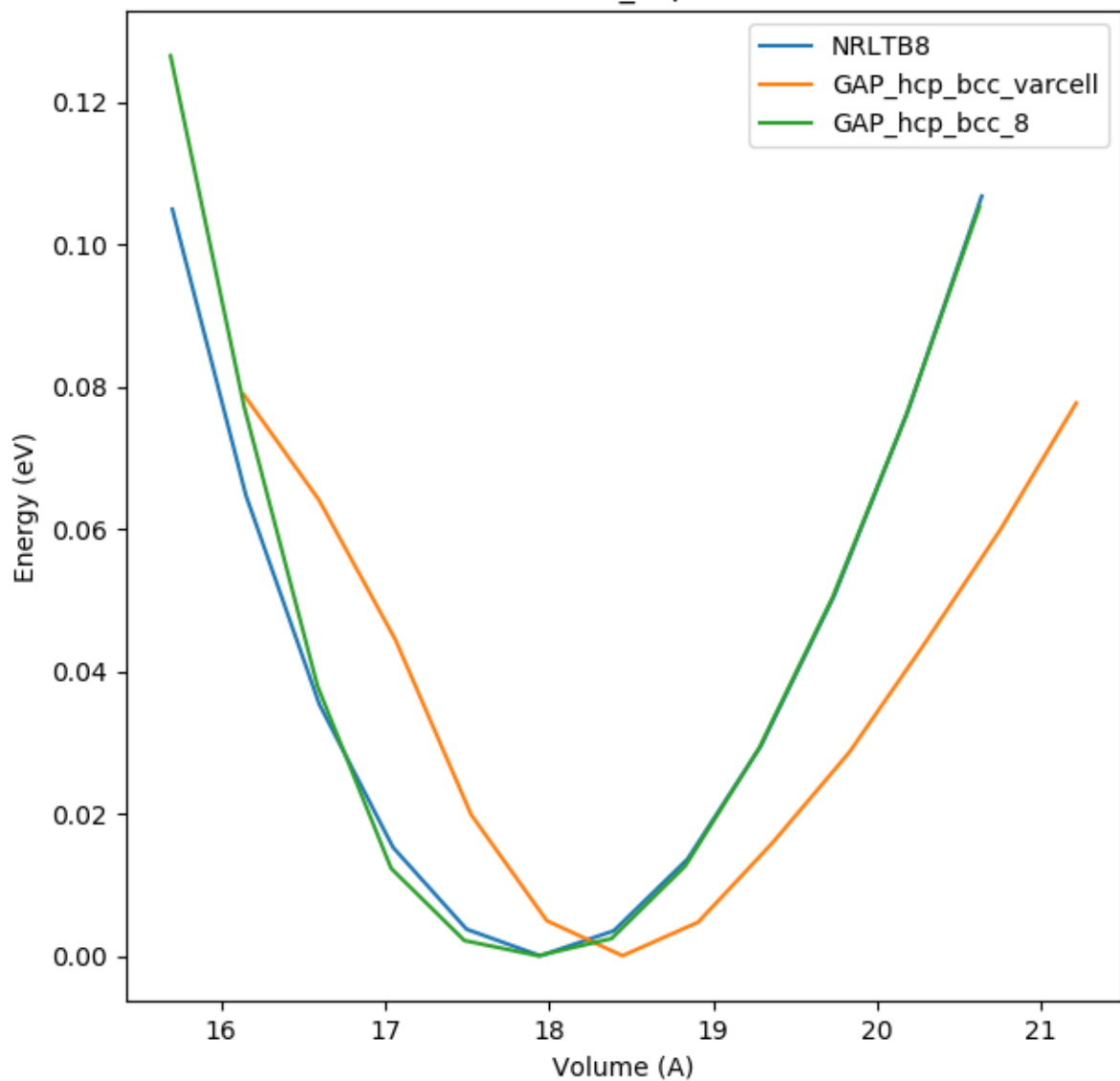
{'hcp_1000K': 4, 'bcc_500K': 4, 'hcp_500K': 4, 'bcc_1000K': 4, 'hcp_50K': 4, 'bcc_50K': 4}

	-	GAP_hcp_bcc_8	GAP_hcp_bcc_varcell	NRLTB8
0	bcc_c12	121.26	-82%	-20%
1	bcc_c11	180.88	-61%	-34%
2	bcc_c44	55.72	-59%	-51%
3	hcp_c44	4.06	1866%	707%
4	hcp_c13	98.81	-19%	-33%
5	hcp_c12	120.23	-32%	-28%
6	hcp_c11	57.19	320%	155%
7	hcp_c66	-45.75	-291%	-202%
8	hcp_c33	328.47	-41%	-45%

bulk_bcc

bulk_hcp

NRLTB8
GAP_hcp_bcc_varcell
GAP_hcp_bcc_8

surface-decohesion-100-unrelaxed

surface-decohesion-110-unrelaxed

surface-decohesion-111-unrelaxed