## GAP\_fd16

<command\_line><![CDATA[ at\_file=Ti\_hcp\_bcc16.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=200 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\_fdcell.xml default\_sigma={0.0001 0.05 0.05 0.0}]]>

{'hcp\_fdcell': 216, 'bcc\_fdcell': 162}

	-	NRLTB16	$GAP_{fd16}$
0	bcc_c12	100.20	-44%
1	$bcc\_c11$	105.31	-3%
2	$bcc_c44$	38.92	192%
3	$hcp_c44$	34.28	140%
4	$hcp_c13$	68.39	-2%
5	$hcp_c12$	57.67	-151%
6	$hcp_c11$	176.57	-6%
7	$hcp\_c66$	56.05	86%
8	$hcp_c33$	171.23	56%













