

Results using eam88 on a linux machine

Energy: eV/atom

Volume: Å<sup>3</sup>/atom

Distance: Å

All calculations fully relaxed at 0 K

**Ni**

fcc	10.9036 final	volume	
fcc	-4.4500 final	potential	energy
hcp	11.1246 final	volume	
hcp	-4.4374 final	potential	energy
hcp	2.4796 final	a	
hcp	4.1786 final	c	
hcp	1.6852 final	c/a	
bcc	11.7695 final	volume	
bcc	-4.3736 final	potential	energy
DC	15.6022 final	volume	
DC	-3.1017 final	potential	energy
SC	13.2943 final	volume	
SC	-3.9750 final	potential	energy

**Al**

fcc	16.6075 final	volume	
fcc	-3.3600 final	potential	energy
hcp	17.3044 final	volume	
hcp	-3.3480 final	potential	energy
hcp	2.8109 final	a	
hcp	5.0579 final	c	
hcp	1.7994 final	c/a	
bcc	19.0970 final	volume	
bcc	-3.2734 final	potential	energy
DC	22.3782 final	volume	
DC	-2.9243 final	potential	energy
SC	19.7934 final	volume	
SC	-3.3111 final	potential	energy

**H**

dimer	-2.3695 final	potential	energy
dimer	0.7396 final	bond	length

**Ni-Al**

B1	11.7335 final	volume	
B1	-4.4254 final	potential	energy
B1	2.8630 final	a	
B1	2.8630 final	c	
B1	1.0000 final	c/a	
L12(Ni3Al)	11.3524 final	volume	
L12(Ni3Al)	-4.5983 final	potential	energy

**Ni-H**

1H fcc Oh	256 Ni + 1 H		
1H fcc Oh	10.8743 final	volume	
1H fcc Oh	-4.4412 final	potential	energy

**Al-H**

1H fcc Oh	256 Al + 1 H		
1H fcc Oh	16.5630 final	volume	
1H fcc Oh	-3.3537 final	potential	energy