

Surface (100)

Property	GAP	VASP	Dragoni	Espresso	Exp.
E_{100}^f (J/m ²)	2.642	2.638	2.547	2.543	-
Δ_{12} (%)	-3.354	-0.032	-0.455	-	-5±2
Δ_{23} (%)	1.779	2.033	1.662	-	5±2
Δ_{34} (%)	0.285	-0.851	-0.487	-	-

Surface (100)

System	n systems	n atoms per system	n atoms total	error
isolated atom	1	1	1	0.08 meV
dimer	40	2	80	0.31 meV/atom
bcc distorted	547	2	1094	0.31 meV/atom
bcc phonon	50	54	2700	0.19 meV/atom
vacancy	30	53	1590	0.52 meV/atom
di-vacancy	35	126	4410	0.10 meV/atom
tri-vacancy	15	117	1755	0.10 meV/atom
SIA	25	129	3225	0.03 meV/atom
liquids	58	128	7424	1.78 meV/atom
short_range	50	55	2750	6.26 meV/atom
surf 100	20	12	240	3.56 meV/atom
surf 110	20	12	240	- meV/atom
total	891	-	25509	

Bain path

