Contents

1 Narrowed Data for Sasha

1.0.1 Objective Function

PARAMETERS fdd=0.1958363809 qdds=0.5591275855 qddp=0.5690351902 qddd=0.7745947522 b0=58.0906936439 p0=1.2185323579 b1=-3.2299188646 p1=0.6862915307 b2=593519.1134129359 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.0474400934 cr3=-1.2317472193 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18 VARGS -vfdd=0.1958363809 -vqdds=0.5591275855 -vqddp=0.5690351902 -vqddd=0.7745947522 -vb0=58.0906936439 -vp0=1.2185323579 -vb1=-3.2299188646 -vp1=0.6862915307 -vb2=593519.1134129359 -vm2=-11.5000000000 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.0474400934 -vcr3=-1.2317472193 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrmaxhm=10.1000000000

Quantity	From Model	Target
a_{hcp}	5.58523112	5.57678969
c/a	1.58371266	1.58731122
a_{omega}	8.93475285	8.73254342
c_{omega}	5.38726911	5.32343103
a_{4h}	5.57584691	5.56325146
c_{4h}	18.09810672	17.75908031
a_{6h}	5.57365569	5.54639384
c_{6h}	27.18378460	26.77136353
a_{bcc}	6.20079768	6.17948863
a_{fcc}	7.87290654	7.88677000
DE(o,h)	0.58764167	-0.63343333
DE(4h,h)	1.58019500	3.17160000
DE(6h,h)	2.48264833	3.72005000
DE(b,h)	5.35128500	7.63520000
DE(f,h)	3.78088500	4.51880000
c_{11}	171.60928873	176.10000000
c_{33}	198.90063708	190.50000000
c_{44}	47.42549704	50.80000000
c_{12}	94.65941969	86.90000000
c_{13}	61.22624060	68.30000000
M_{freq0}	2.59341377	2.85858719
M_{freq1}	2.59341378	2.85858719
M_{freq2}	2.59341378	2.85858719
M_{freq3}	2.59341379	2.85858719
M_{freq4}	5.85272461	5.66706047
M_{freq5}	5.85272461	5.66706047
H_{freq0}	3.82320403	4.80643423
H_{freq1}	3.82320403	5.58010025
H_{freq2}	6.40288977	5.65316738
H_{freq3}	6.40288977	6.36651842
H_{freq4}	7.92857431	6.40050186
H_{freq5}	7.92857431	7.64082373
bandw. G	3.69394702	5.87085872
bandw. K	4.65178817	4.97424321
bandw. M	5.19329495	7.78109872
bandw. L	4.21232412	6.34433701
bandw. H	3.54700549	9.70902614
$DOSerr_h$	0.00000000	0.00000000
$DOSerr_o$	0.00000000	0.00000000
E_{prisf}	98.95340236	220.00000000

——— $E_{prismaticfault}$ ———

tbe:	98.953	mJ/m^2	
DFT:	250.000	mJ/m^2	[Benoit 2012]
DFT:	233.000	mJ/m^2	[Ackland 1999]

——— $E_{Basalfault}$ I2 ———

tbe:	211.658	mJ/m^2	
DFT:	260.000	mJ/m^2	[Benoit 2012]

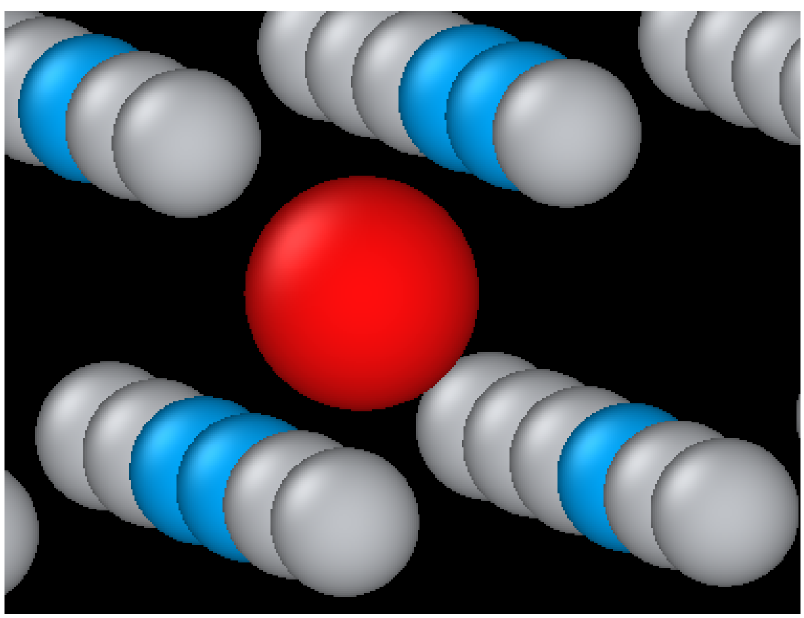
1.0.2 Defect Clusters

——— $E_{vacancyformation}$ ———

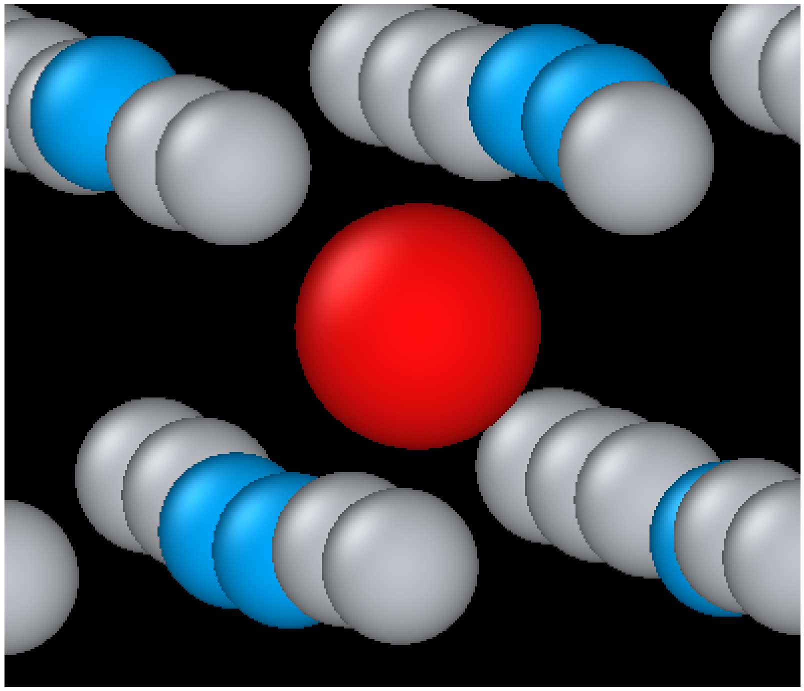
tbe:	2.347 eV	
DFT:	1.950 eV	GGA-PAW: Angsten (2013)
exp:	1.270 eV	Hashimoto (1984)

1. Octahedral O interstitial relaxation

   Initial:

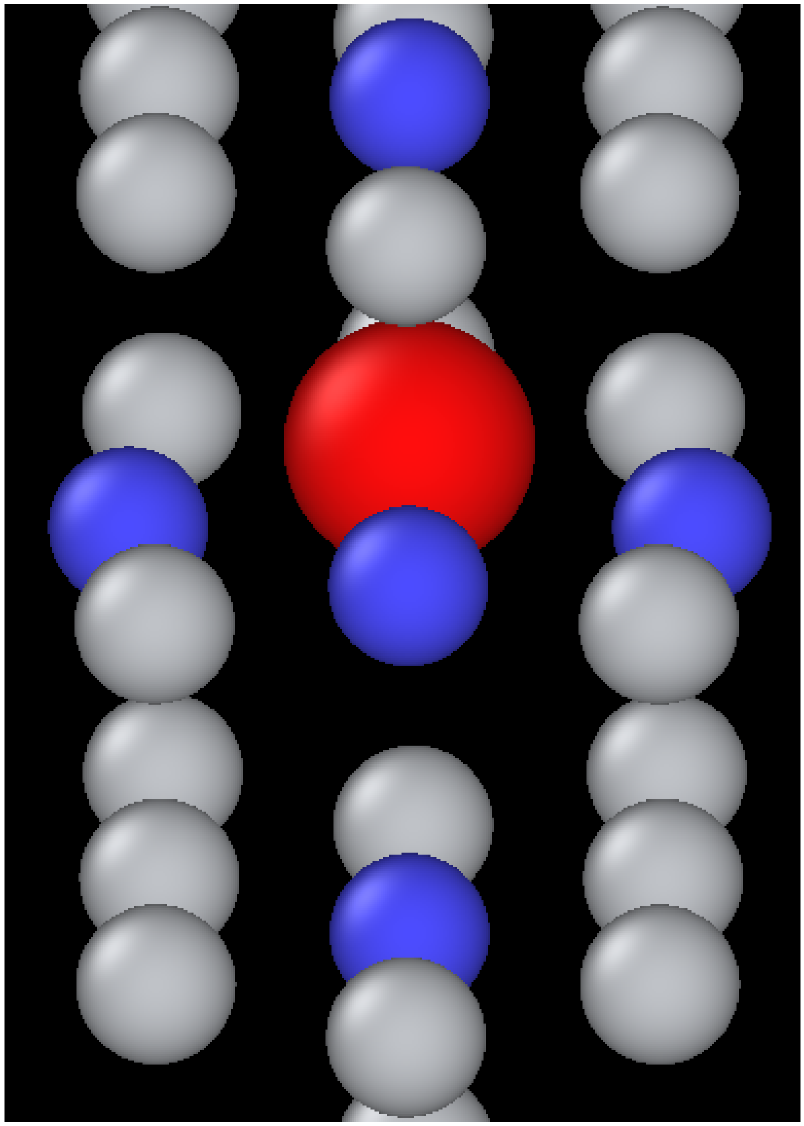
   

   Final:

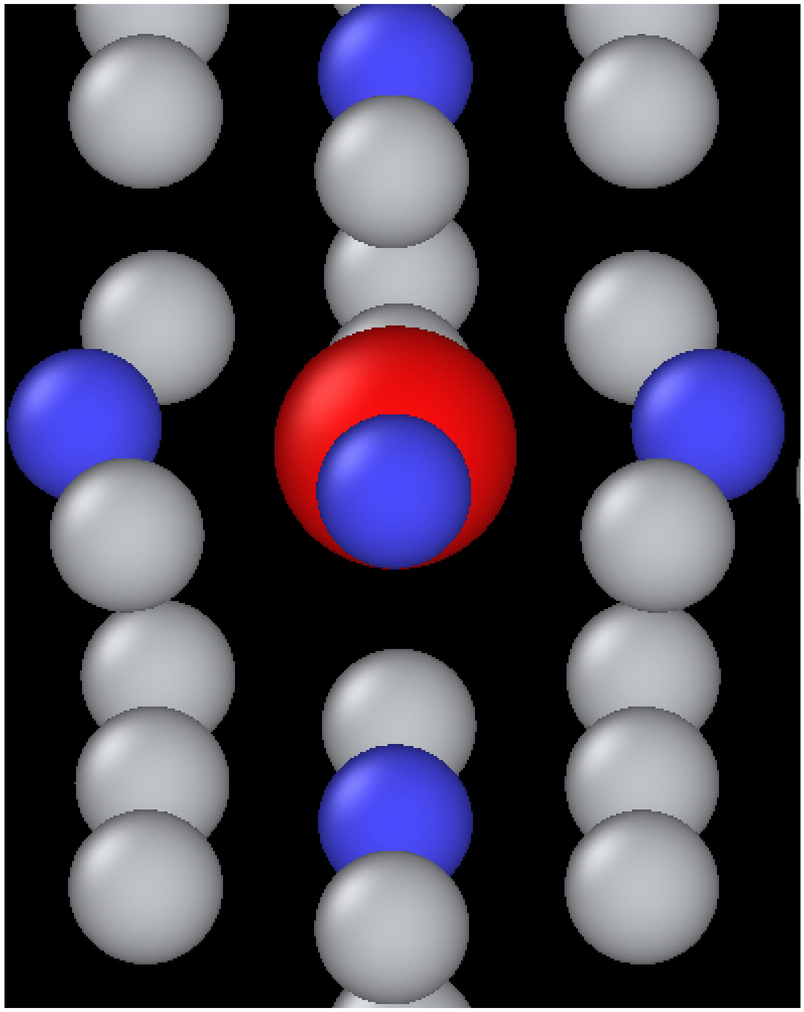


2. Tetrahedral O interstitial relaxation

   Initial:



Final:



3. Energies for defects

   Relative differences are

   » ($E_{tetrahedral}$ - $E_{octahedral}$)

tbe:	1.65 eV	
GGA-DFT:	1.23 eV	Kwasniak (2013)

   » ($E_{hexahedral}$ - $E_{octahedral}$)

   tbe: 0.90 eV

$>$ Note: Preference for tetrahedral oxygen to go into hexahedral site as seen by images above

All formation energies below use the chemical potential of Akysonov (2013) of value $\mu_{\text{oxygen}} = \frac{5.6}{2} eV$.

4. All formation energies

Quantity	Energy (eV)
Ef_{Vf}	2.347
Ef_{Tsol}	- 21.783
$Ef_{Tdilimp}$	- 28.991
$Ef_{Tformation}$	- 21.783
$Ef_{TVformation}$	- 18.905
$Ef_{Tvacsolbind}$	- 0.530
Ef_{Osol}	- 23.436
$Ef_{Odilimp}$	- 30.645
$Ef_{Oformation}$	- 23.436
$Ef_{OVformation}$	- 18.905
$Ef_{Ovacsolbind}$	- 2.183
Ef_{OOsol}	- 49.606
$Ef_{OOdilimp}$	- 56.814
$Ef_{OOformation}$	- 46.806
$Ef_{OOVformation}$	- 41.910
$Ef_{OOvacsolbind}$	- 2.547
Ef_{OOOsol}	- 76.037
$Ef_{OOOdilimp}$	- 83.246
$Ef_{OOOformation}$	- 70.437
$Ef_{OOOVformation}$	- 66.013
$Ef_{OOOvacsolbind}$	- 2.076
$Ef_{OOOOsol}$	- 102.470
$Ef_{OOOOdilimp}$	- 109.679
$Ef_{OOOOformation}$	- 94.070
$Ef_{OOOOVformation}$	- 88.998
$Ef_{OOOOvacsolbind}$	- 2.724
$Ef_{OOOOOsol}$	- 128.781
$Ef_{OOOOOdilimp}$	- 135.989
$Ef_{OOOOOformation}$	- 117.581
$Ef_{OOOOOVformation}$	- 113.649
$Ef_{OOOOOvacsolbind}$	- 1.583
$Ef_{OOOOOOsol}$	- 155.148
$Ef_{OOOOOOdilimp}$	- 162.357
$Ef_{OOOOOOformation}$	- 141.148
$Ef_{OOOOOOVformation}$	- 137.110
$Ef_{OOOOOOvacsolbind}$	- 1.690

1.0.3 Gamma surfaces

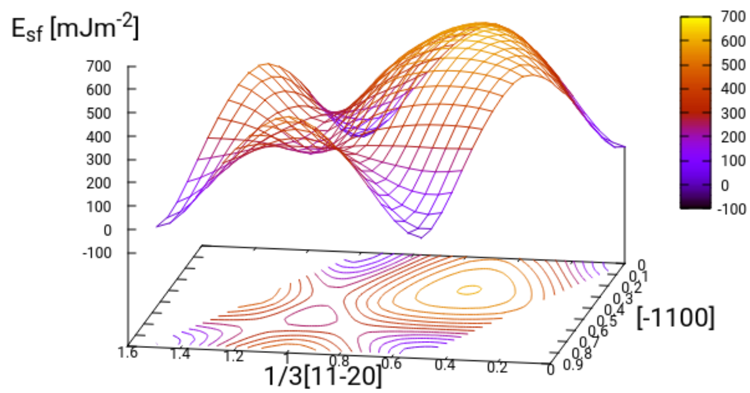
Energies are accurate to within 2 mJm^{-2}, comparing the energies of points in the corners which (the zeros of energy). So surface energies might be ± 2 mJm^{-2} off which is reasonable.

These calculations were done in tight binding with 15 layers for both basal and prismatic with k-points adjusted accordingly. DFT comparisons are usind results of Rodney.

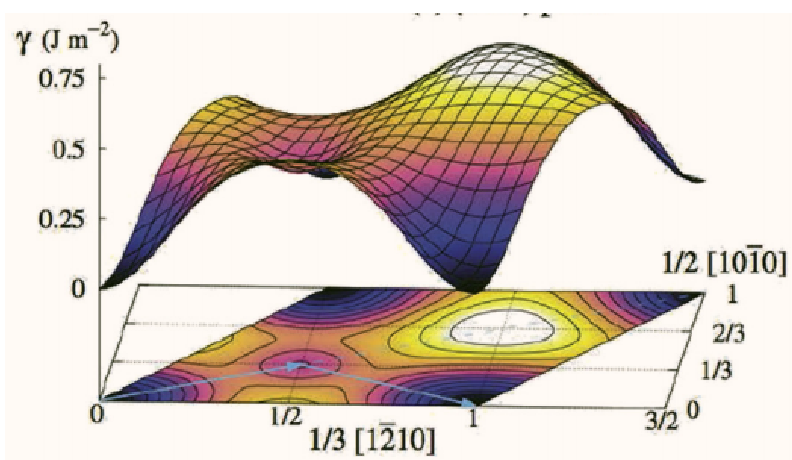
The Pyramidal surface was obtained using the same 32 atom cell that Ready used in his paper on the pyramidal gamma surface with DFT pseudopotentials.

1. Basal

   TBE:

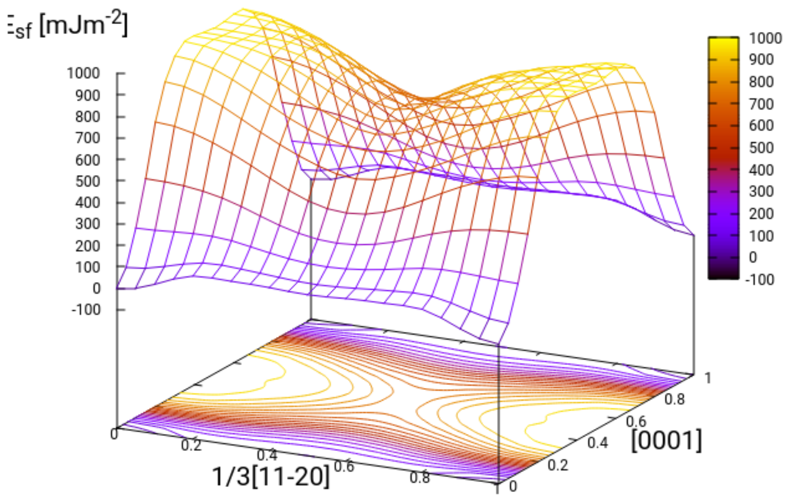


   DFT:

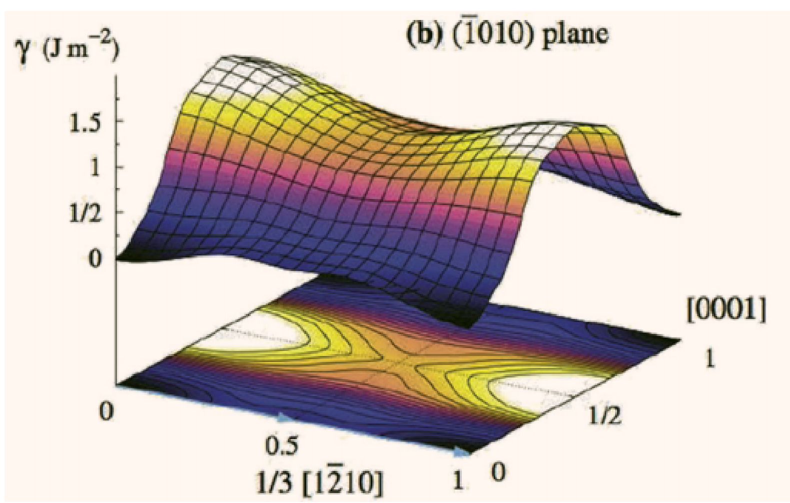


2. Prismatic

   TBE:

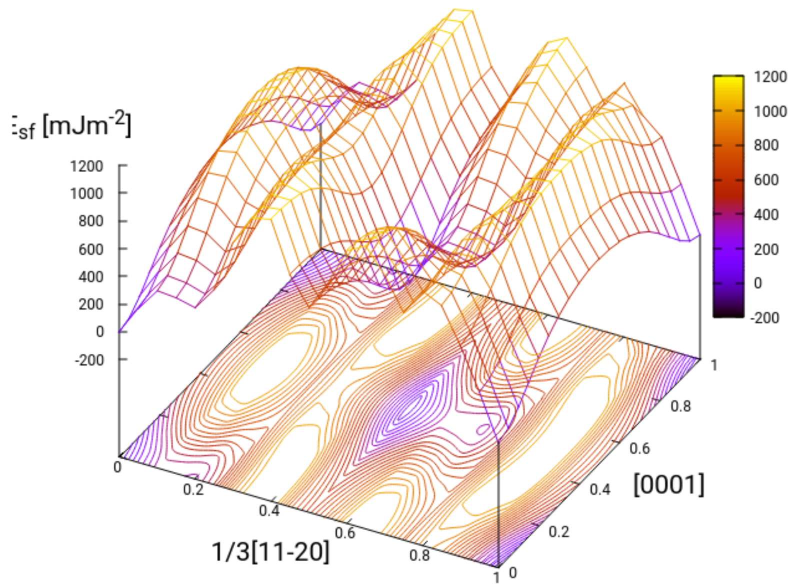


DFT:

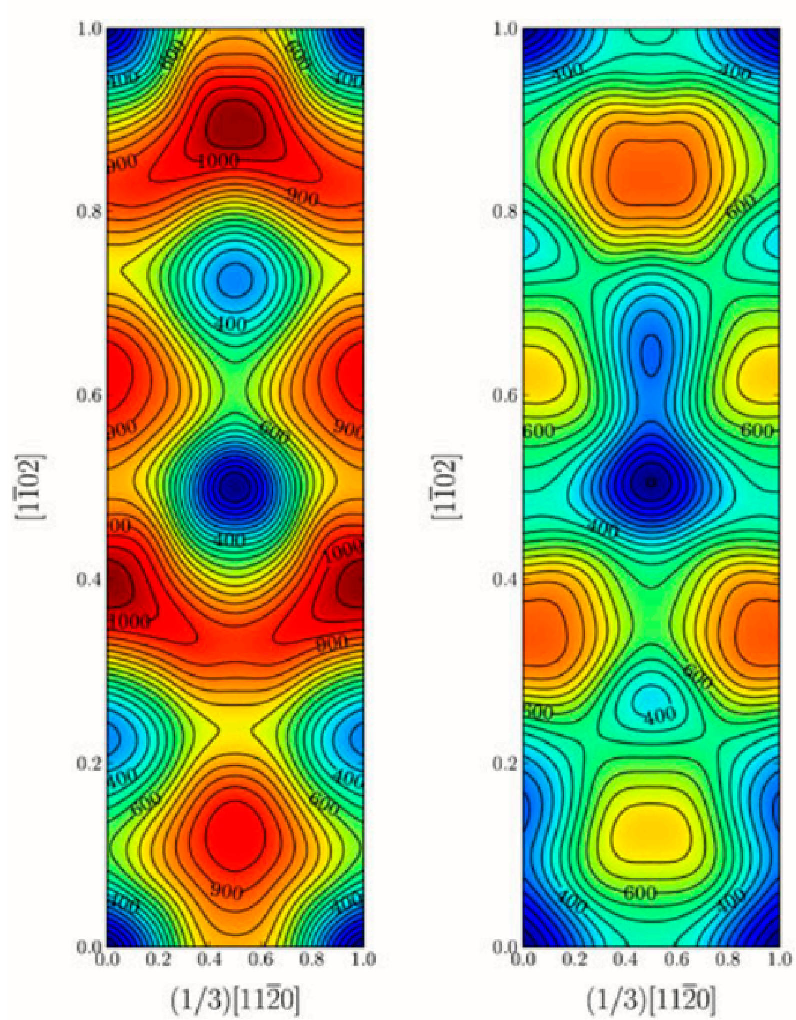


3. Pyramidal first order

   TBE:



DFT pseudopot:



4. Data $\text{basal}_{\text{gsdata}}$ $\text{prismatic}_{\text{gsdata}}$ $\text{pyramidal}_{\text{gsdata}}$

1.0.4 Dislocation core structures

"Images/""ddplot_IP1_noo_best_model_alat"-eps-converted-to.pdf

"Images/""ddplot_IP2_noo_best_model_alat"-eps-converted-to.pdf

"Images/""ddplot_IP3_noo_best_model_alat"-eps-converted-to.pdf

"Images/""ddplot_IP4_noo_best_model_alat"-eps-converted-to.pdf

"Images/""ddplot_IP5_noo_best_model_alat"-eps-converted-to.pdf

1. Data IP1 IP2 IP3 IP4 IP5

1.0.5 Directory of the results

file:///home/tigany/Documents/ti/2019-09-11_final_model/tbe/dislocations/2019-11-08_no_omega_ordering_ec_latpar/ file:///home/tigany/Documents/ti/final_model_2019-11

1.0.6 BOP

1. 4 recursion levels

   kbT = 0.1

   » Lattice parameters:

   > hcp

a	2.901660 Å
c	4.747485 Å
etot	-18.342162 eV

> omega

a	7.917318 Å
c	2.749892 Å
etot	-17.458700 eV

Omega is still not as stable as hcp as expected from model.

» Elastic Constants

Quantity	calc. (10^{11} Pa)	exp. (10^{11} GPa)
C11	1.781	1.761
C12	0.738	0.868
C13	0.611	0.682
C33	1.969	1.905
C44	0.285	0.508
C66	0.522	0.450
K	1.050	1.101
R	0.669	0.618
H	0.558	0.489