things-to-do

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Contents

1 TODO Titanium Optimisation

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START: OBJECTIVE FUNCTION

ti_obj_weights.py
 starting..
   ext = ti ,
   file = fmin.val ,
   vals =  fdd=0.1174466123 qdds=0.3974516540 qddp=0.3909616843 qddd=0.4513787662 b0=12
6 r1=1.0308550249 rc=1.2000213349 cr3=-1.0000000000 rmaxh=1.2120215483 b1=0.0000000000
   binaries in /opt/lmto/bld7.13.0/openmpi/3.1.0/intel/14.0.1/o



Obtaining Bandwidth and optimising c and a

    Bandwidth Scaling routine

nbands = 18, ef = 0.02977, ncol = 2
Bandwidth at Gamma:
   TBE:    5.916 eV
   DFT:    5.900 eV


Getting hcp c/a
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```
Using Nelder-Mead

Optimization terminated successfully.
 Current function value: -0.684831
 Iterations: 28
 Function evaluations: 64
Got a, c : a=5.4161008400, c=8.8279655592 c/a=1.6299485220. Volume per atom=112.133337
Targets  : a=5.5767896900, c=8.8521008200 c/a=1.5873112152. Volume per atom=119.210777

Getting hcp shear constants ...

 C_11 =    122.335 GPa

 C_33 =    124.303 GPa

 C_44 =     42.309 GPa

 C_66 =     44.277 GPa

 C_12 =     33.618 GPa

 C_13 =     33.782 GPa

shear constants: c_11=122.3, c_33=124.3, c_44= 42.3, c_12= 33.6, c_13= 33.8, c_66=  44
 target: c_11=176.1, c_33=190.5, c_44= 50.8, c_12= 86.9, c_13= 68.3, c_66=  44.6, S= 73

   bulk modulus: 63; target: 110

Obtaining frequencies for M and H points in hcp Brillouin zone

M frequencies tbe (THz) =  2.5331326195  2.5331326290  2.5331326290  2.5331326386  3.82
M frequencies LDA (THz) =  2.8585871860  2.8585871860  2.8585871860  2.8585871860  5.66

H frequencies tbe (THz) =  1.5399197708  1.5399197708  1.8398976627  1.8398976627  3.96
H frequencies LDA (THz) =  4.8064342322  5.5801002486  5.6531673769  6.3665184154  6.40

Obtaining bcc Ti quantities

  trial bcc output from pfit = 0.0
  VF = 0.825226
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  Epp bcc = 3.71884
Get hcp - fcc energy difference ..
Using Nelder-Mead

Optimization terminated successfully.
 Current function value: -0.336410
 Iterations: 14
 Function evaluations: 30
 fcc minimum lattice parameter
  a_fcc = 7.676507,  a_fcc_exp = 7.886770
E_fcc - E_hcp = 6.006mRy per atom

Getting omega phase lattice constants and internal parameter ...
Using Nelder-Mead

Optimization terminated successfully.
 Current function value: -1.029450
 Iterations: 27
 Function evaluations: 58

Got omega : a=8.4761, c=5.4016 c/a=0.6373, using u=1.0000. Volume per atom=112.0287
Targets   : a=8.7325, c=5.3234 c/a=0.6096, using u=1.0000. Volume per atom=117.1878
bcc:     a=  5.82, K=378 Volume per atom=98
target:  a=  6.18, K=118,
E_bcc - E_hcp = 82.515mRy per atom


 Build Objective Function
     ... With Elastic Net Regularisation
parameter names       fdd     qdds     qddp     qddd       b0       p0      ndt      c
parameter values    0.117    0.397    0.391    0.451   12.420    1.103    2.028   -6.2
  p_norm    0.509    1.722    1.694    1.955   53.802    4.778    8.785   26.900   17.

Total p_norm = 121.68857


 Quantity      predicted    target     norm_pred   norm_tar    sq diff.      weight
-------------------------------------------------------------------------------------
 a_hcp   :   5.41610084   5.57678969   5.41610084   5.57678969   0.02582091 1000.00000
 c_hcp   :   8.82796556   8.85210082   8.82796556   8.85210082   0.00058251 1000.00000
```

c_11 :	122.33537796	176.10000000	1.86500000	2.85408495	0.97828904	1.000000
c_33 :	124.30323926	190.50000000	1.89500000	3.08746839	1.42198086	1.000000
c_44 :	42.30901811	50.80000000	0.64500000	0.82332490	0.03179977	1.000000
c_12 :	33.61763067	86.90000000	0.51250000	1.40840422	0.80264436	1.000000
c_13 :	33.78161911	68.30000000	0.51500000	1.10695061	0.35040552	1.000000
a_omega :	8.47612090	8.73254342	8.47612090	8.73254342	0.06575251	10.000000
c_omega :	5.40164179	5.32343103	5.40164179	5.32343103	0.00611692	10.000000
DE(o,h) :	-0.73462833	-0.73475386	-0.73462833	-0.73475386	0.00000002	10.000000
DE(f,h) :	6.00578500	6.60015000	6.00578500	6.60015000	0.35326975	10.000000
a_bcc :	5.81618924	6.17948863	5.81618924	6.17948863	0.13198645	5.000000
M_freq_0:	2.53313262	2.85858719	2.53313262	2.85858719	0.10592067	0.100000
M_freq_1:	2.53313263	2.85858719	2.53313263	2.85858719	0.10592067	0.100000
M_freq_2:	2.53313263	2.85858719	2.53313263	2.85858719	0.10592067	0.100000
M_freq_3:	2.53313264	2.85858719	2.53313264	2.85858719	0.10592066	0.100000
M_freq_4:	3.82569593	5.66706047	3.82569593	5.66706047	3.39062338	0.100000
M_freq_5:	3.82569593	5.66706047	3.82569593	5.66706047	3.39062338	0.100000
H_freq_0:	1.53991977	4.80643423	1.53991977	4.80643423	10.67011673	0.100000
H_freq_1:	1.53991977	5.58010025	1.53991977	5.58010025	16.32305829	0.100000
H_freq_2:	1.83989766	5.65316738	1.83989766	5.65316738	14.54102591	0.100000
H_freq_3:	1.83989766	6.36651842	1.83989766	6.36651842	20.49029544	0.100000
H_freq_4:	3.96697370	6.40050186	3.96697370	6.40050186	5.92205930	0.100000
H_freq_5:	3.96697370	7.64082373	3.96697370	7.64082373	13.49717403	0.100000
a_fcc :	7.67650748	7.88677000	7.67650748	7.88677000	0.04421033	5.000000
bw at G :	5.91588880	5.89956160	5.91588880	5.89956160	0.00026658	100.000000

Objective function: 1657010