things-to-do

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Contents

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START: OBJECTIVE FUNCTION

ti_obj_new_ec_cutoffs_canon.py
 starting..
   ext = ti ,
   file = fmin.val ,
   vals = fdd=0.1737703199 qdds=0.5706158058 qddp=0.6421834099 qddd=0.7560903882
          b0=278.8444422514 p0=1.7961642354 b1=0.0000000000 p1=0.000000000
          ndt=1.9624397374 cr1=-6.9348461726 cr2=4.0612686987 cr3=-1.0000000000
          r1=0.9819448403 rc=1.3464870767 rmaxh=1.3599519474
   binaries in /opt/lmto/bld7.13.0/openmpi/3.1.0/intel/14.0.1/o



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

Optimization terminated successfully.
         Current function value: -0.333512
         Iterations: 29
         Function evaluations: 60
Got a, c : a=5.5401081318, c=8.9583629249 c/a=1.6170014577. Volume per atom=119.059970
Targets  : a=5.5767896900, c=8.8521008200 c/a=1.5873112152. Volume per atom=119.210777

Obtaining Bandwidth

  eval 1 for bandwidth = -0.1587
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  eval 2 for bandwidth = 0.129
bandwidth: 0.288 (target: 0.426)

Getting hcp shear constants ...

 C_11 =    177.624 GPa

 C_33 =    191.588 GPa

 C_44 =     46.334 GPa

 C_12 =     88.164 GPa

 C_13 =     67.996 GPa

shear constants: c_11=177.6, c_33=191.6, c_44= 46.3, c_12= 88.2, c_13= 68.0, 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
   bulk modulus: 111; target: 110

Obtaining bcc Ti quantities

  trial bcc output from pfit = 0.0
  VF = 0.943542
  Epp bcc = 0.491615

Getting omega phase lattice constants and internal parameter ...

Using Nelder-Mead

Optimization terminated successfully.
         Current function value: -0.498206
         Iterations: 38
         Function evaluations: 81

Got omega : a=8.7091, c=5.4026 c/a=0.6203, u=1.0001. Volume per atom=118.2943
Targets   : a=8.7325, c=5.3234 c/a=0.6096, u=1.0000. Volume per atom=117.1878
E_omega - E_hcp = 0.687mRy per atom
      GGA Target: -0.735
bcc:     a=  6.08, K=57 Volume per atom=112
target:  a=  6.18, K=118,
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       E_bcc - E_hcp = 19.358mRy per atom


 Build Objective Function

                     predicted       target
  a_hcp       :    5.54010813     5.57678969
  c_hcp       :    8.95836292     8.85210082
  c_11        :  177.62375172   176.10000000
  c_33        :  191.58842280   190.50000000
  c_44        :   46.33439251    50.80000000
  c_12        :   88.16405241    86.90000000
  c_13        :   67.99572101    68.30000000
  a_omega     :    8.70914358     8.73254342
  c_omega     :    5.40260729     5.32343103
  u_omega     :    1.00009549     1.00000000
  DE (o, hcp) :    0.68707833    -0.73475386
  a_bcc       :    6.08183509     6.17948863
  bandwidth   :    0.28770000     0.42600000

Objective function: 431
```