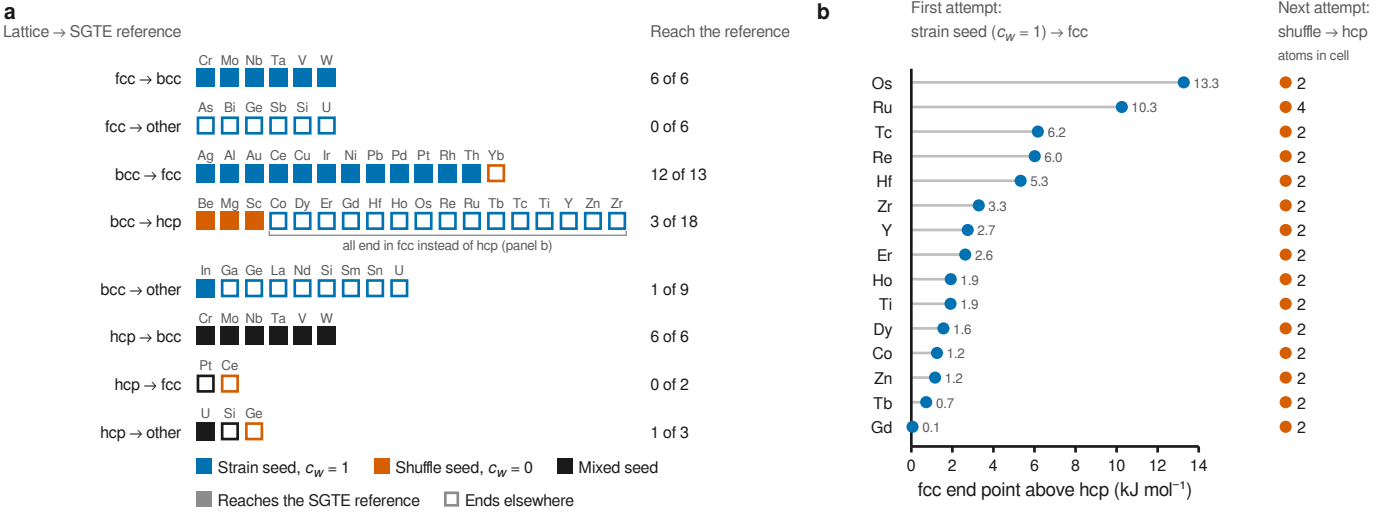
a
Lattice → SGTE reference
Reach the reference
fcc → bcc
Cr Mo Nb Ta V W
6 of 6
fcc → other
As Bi Ge Sb Si U
0 of 6
bcc → fcc
Ag Al Au Ce Cu Ir Ni Pb Pd Pt Rh Th Yb
12 of 13
bcc → hcp
Be Mg Sc Co Dy Er Gd Hf Ho Os Re Ru Tb Tc Ti Y Zn Zr
3 of 18
all end in fcc instead of hcp (panel b)
bcc → other
In Ga Ge La Nd Si Sm Sn U
1 of 9
hcp → bcc
Cr Mo Nb Ta V W
6 of 6
hcp → fcc
Pt Ce
0 of 2
hcp → other
U Si Ge
1 of 3
Strain seed, $c_w = 1$
Shuffle seed, $c_w = 0$
Mixed seed
Reaches the SGTE reference
Ends elsewhere
b
First attempt:
strain seed ($c_w = 1$) → fcc
Next attempt:
shuffle → hcp
atoms in cell
Os 13.3 2
Ru 10.3 4
Tc 6.2 2
Re 6.0 2
Hf 5.3 2
Zr 3.3 2
Y 2.7 2
Er 2.6 2
Ho 1.9 2
Ti 1.9 2
Dy 1.6 2
Co 1.2 2
Zn 1.2 2
Tb 0.7 2
Gd 0.1 2
0 2 4 6 8 10 12 14
fcc end point above hcp (kJ mol^{-1})