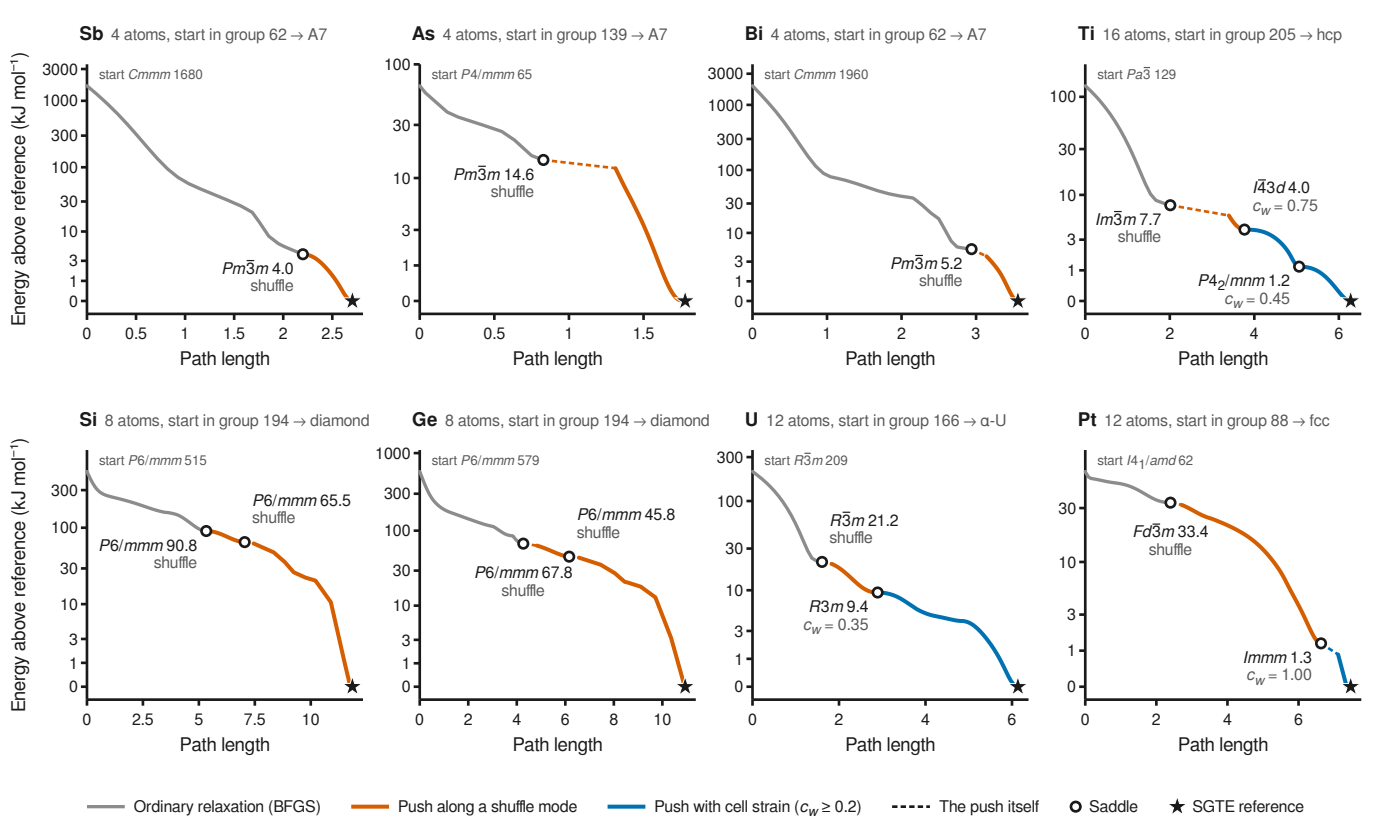
Sb 4 atoms, start in group 62 → A7
start Cmmm 1680
Pm3̄m 4.0
shuffle
As 4 atoms, start in group 139 → A7
start P4/mmm 65
Pm3̄m 14.6
shuffle
Bi 4 atoms, start in group 62 → A7
start Cmmm 1960
Pm3̄m 5.2
shuffle
Ti 16 atoms, start in group 205 → hcp
start Pa3̄ 129
Im3̄m 7.7
shuffle
Ia3̄d 4.0
c_w = 0.75
P4_2/mnm 1.2
c_w = 0.45
Si 8 atoms, start in group 194 → diamond
start P6/mmm 515
P6/mmm 65.5
shuffle
P6/mmm 90.8
shuffle
Ge 8 atoms, start in group 194 → diamond
start P6/mmm 579
P6/mmm 45.8
shuffle
P6/mmm 67.8
shuffle
U 12 atoms, start in group 166 → α-U
start R3̄m 209
R3̄m 21.2
shuffle
R3m 9.4
c_w = 0.35
Pt 12 atoms, start in group 88 → fcc
start I4_1/amd 62
Fd3̄m 33.4
shuffle
Immm 1.3
c_w = 1.00
Energy above reference (kJ mol⁻¹)
Path length
Ordinary relaxation (BFGS)
Push along a shuffle mode
Push with cell strain (c_w ≥ 0.2)
The push itself
Saddle
SGTE reference