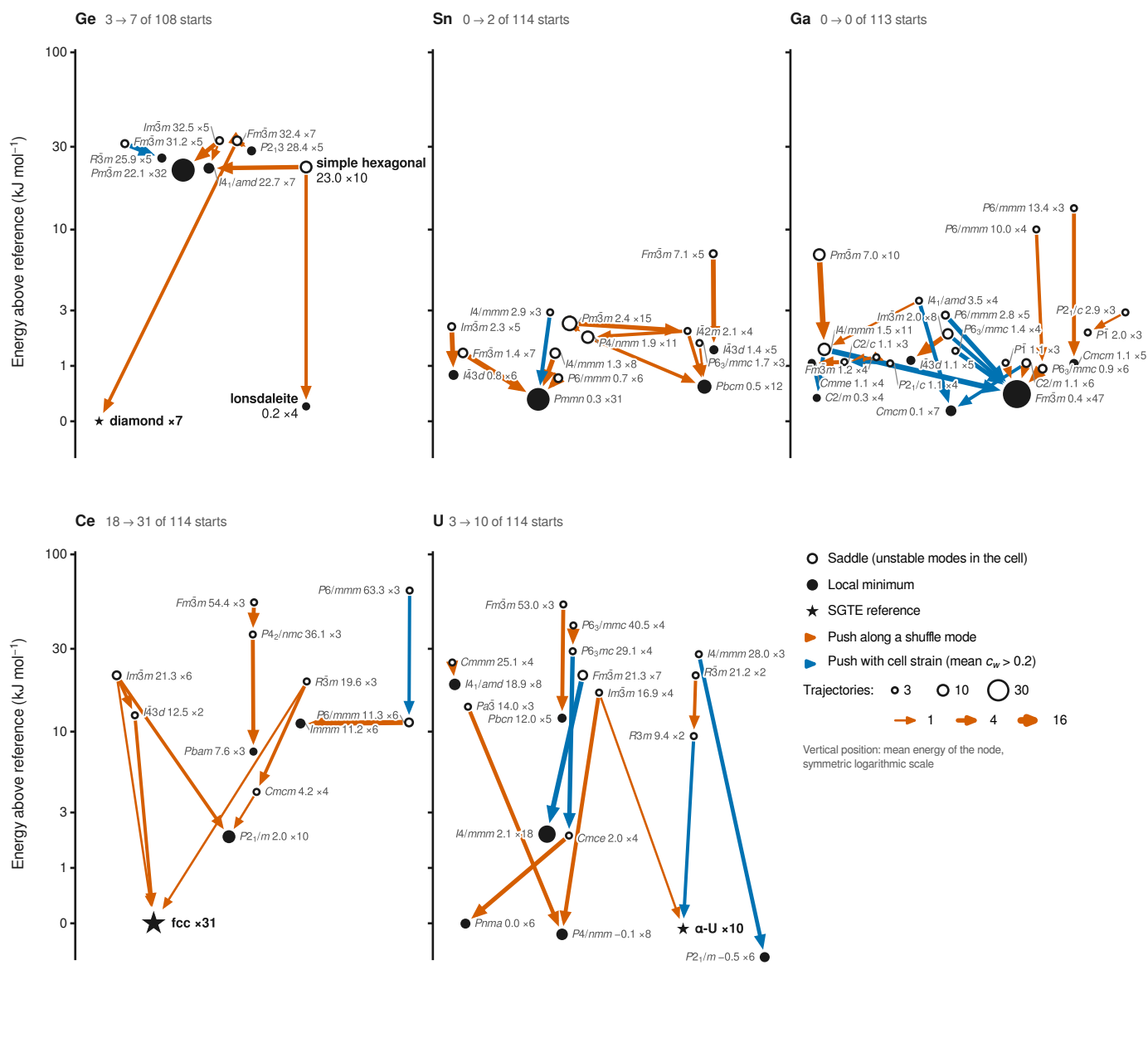
Ge 3 → 7 of 108 starts
Sn 0 → 2 of 114 starts
Ga 0 → 0 of 113 starts
Ce 18 → 31 of 114 starts
U 3 → 10 of 114 starts
Energy above reference (kJ mol⁻¹)
100
30
10
3
1
0
Im3̄m 32.5 ×5
Fm3̄m 31.2 ×5
Fm3̄m 32.4 ×7
P2₁3 28.4 ×5
R3̄m 25.9 ×5
Pm3̄m 22.1 ×32
I4₁/amd 22.7 ×7
simple hexagonal
23.0 ×10
diamond ×7
lonsdaleite
0.2 ×4
Fm3̄m 7.1 ×5
I4/mmm 2.9 ×3
Im3̄m 2.3 ×5
Pm3̄m 2.4 ×15
I42̄m 2.1 ×4
P4/nmm 1.9 ×11
Fm3̄m 1.4 ×7
I43̄d 1.4 ×5
I4/mmm 1.3 ×8
P6₃/mmc 1.7 ×3
I43̄d 0.8 ×6
P6/mmm 0.7 ×6
Pbcm 0.5 ×12
Pmmn 0.3 ×31
P6/mmm 13.4 ×3
P6/mmm 10.0 ×4
Pm3̄m 7.0 ×10
I4₁/amd 3.5 ×4
Im3̄m 2.0 ×8
P6/mmm 2.8 ×5
P2₁/c 2.9 ×3
I4/mmm 1.5 ×11
P6₃/mmc 1.4 ×4
P1̄ 2.0 ×3
C2/c 1.1 ×3
P1̄ 1.1 ×3
Fm3̄m 1.2 ×4
I43̄d 1.1 ×5
Cmcm 1.1 ×5
Cmme 1.1 ×4
P2₁/c 1.1 ×4
P6₃/mmc 0.9 ×6
C2/m 1.1 ×6
C2/m 0.3 ×4
Fm3̄m 0.4 ×47
Cmcm 0.1 ×7
Fm3̄m 54.4 ×3
P6/mmm 63.3 ×3
P4₂/nmc 36.1 ×3
Im3̄m 21.3 ×6
R3̄m 19.6 ×3
I43̄d 12.5 ×2
P6/mmm 11.3 ×6
I4/mmm 11.2 ×6
Pbam 7.6 ×3
Cmcm 4.2 ×4
P2₁/m 2.0 ×10
fcc ×31
Fm3̄m 53.0 ×3
P6₃/mmc 40.5 ×4
P6₃mc 29.1 ×4
I4/mmm 28.0 ×3
Cmmm 25.1 ×4
Fm3̄m 21.3 ×7
R3̄m 21.2 ×2
I4₁/amd 18.9 ×8
Im3̄m 16.9 ×4
Pa3̄ 14.0 ×3
Pbcn 12.0 ×5
R3m 9.4 ×2
I4/mmm 2.1 ×18
Cmce 2.0 ×4
Pnma 0.0 ×6
P4/nmm −0.1 ×8
α-U ×10
P2₁/m −0.5 ×6
Saddle (unstable modes in the cell)
Local minimum
SGTE reference
Push along a shuffle mode
Push with cell strain (mean c_w > 0.2)
Trajectories: 3 10 30
1 4 16
Vertical position: mean energy of the node, symmetric logarithmic scale