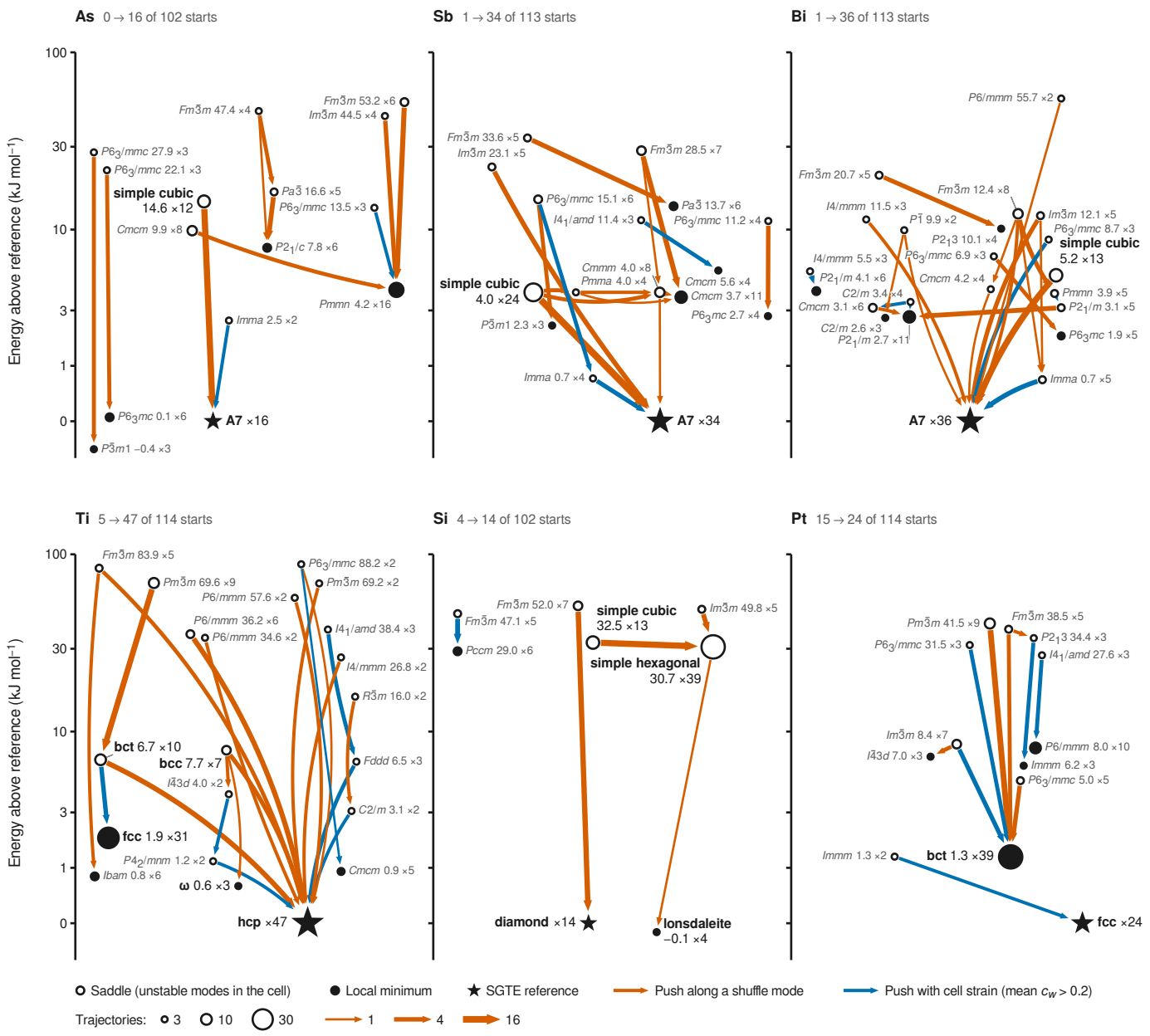
As 0 → 16 of 102 starts
Sb 1 → 34 of 113 starts
Bi 1 → 36 of 113 starts
Ti 5 → 47 of 114 starts
Si 4 → 14 of 102 starts
Pt 15 → 24 of 114 starts
Energy above reference (kJ mol⁻¹)
100
30
10
3
1
0
Fm3̄m 47.4 ×4
Fm3̄m 53.2 ×6
Im3̄m 44.5 ×4
P6₃/mmc 27.9 ×3
P6₃/mmc 22.1 ×3
simple cubic
14.6 ×12
Pa3̄ 16.6 ×5
P6₃/mmc 13.5 ×3
Cmcm 9.9 ×8
P2₁/c 7.8 ×6
Pmmn 4.2 ×16
Imma 2.5 ×2
P6₃mc 0.1 ×6
A7 ×16
P3̄m1 −0.4 ×3
Fm3̄m 33.6 ×5
Im3̄m 23.1 ×5
Fm3̄m 28.5 ×7
P6₃/mmc 15.1 ×6
Pa3̄ 13.7 ×6
I4₁/amd 11.4 ×3
P6₃/mmc 11.2 ×4
Cmmm 4.0 ×8
Pmma 4.0 ×4
simple cubic
4.0 ×24
Cmcm 5.6 ×4
Cmcm 3.7 ×11
P6₃mc 2.7 ×4
P3̄m1 2.3 ×3
Imma 0.7 ×4
A7 ×34
P6/mmm 55.7 ×2
Fm3̄m 20.7 ×5
Fm3̄m 12.4 ×8
I4/mmm 11.5 ×3
P1̄ 9.9 ×2
Im3̄m 12.1 ×5
P6₃/mmc 8.7 ×3
P2₁3 10.1 ×4
simple cubic
5.2 ×13
I4/mmm 5.5 ×3
P6₃/mmc 6.9 ×3
P2₁/m 4.1 ×6
Cmcm 4.2 ×4
C2/m 3.4 ×4
Pmmn 3.9 ×5
Cmcm 3.1 ×6
P2₁/m 3.1 ×5
C2/m 2.6 ×3
P2₁/m 2.7 ×11
P6₃mc 1.9 ×5
Imma 0.7 ×5
A7 ×36
Fm3̄m 83.9 ×5
Pm3̄m 69.6 ×9
P6₃/mmc 88.2 ×2
Pm3̄m 69.2 ×2
P6/mmm 57.6 ×2
P6/mmm 36.2 ×6
P6/mmm 34.6 ×2
I4₁/amd 38.4 ×3
I4/mmm 26.8 ×2
R3̄m 16.0 ×2
bct 6.7 ×10
bcc 7.7 ×7
Fddd 6.5 ×3
I4̄3d 4.0 ×2
C2/m 3.1 ×2
fcc 1.9 ×31
P4₂/mnm 1.2 ×2
Ibam 0.8 ×6
Cmcm 0.9 ×5
ω 0.6 ×3
hcp ×47
Fm3̄m 52.0 ×7
Im3̄m 49.8 ×5
Fm3̄m 47.1 ×5
simple cubic
32.5 ×13
Pccm 29.0 ×6
simple hexagonal
30.7 ×39
diamond ×14
lonsdaleite
−0.1 ×4
Pm3̄m 41.5 ×9
Fm3̄m 38.5 ×5
P6₃/mmc 31.5 ×3
P2₁3 34.4 ×3
I4₁/amd 27.6 ×3
Im3̄m 8.4 ×7
I4̄3d 7.0 ×3
P6/mmm 8.0 ×10
Immm 6.2 ×3
P6₃/mmc 5.0 ×5
Immm 1.3 ×2
bct 1.3 ×39
fcc ×24
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