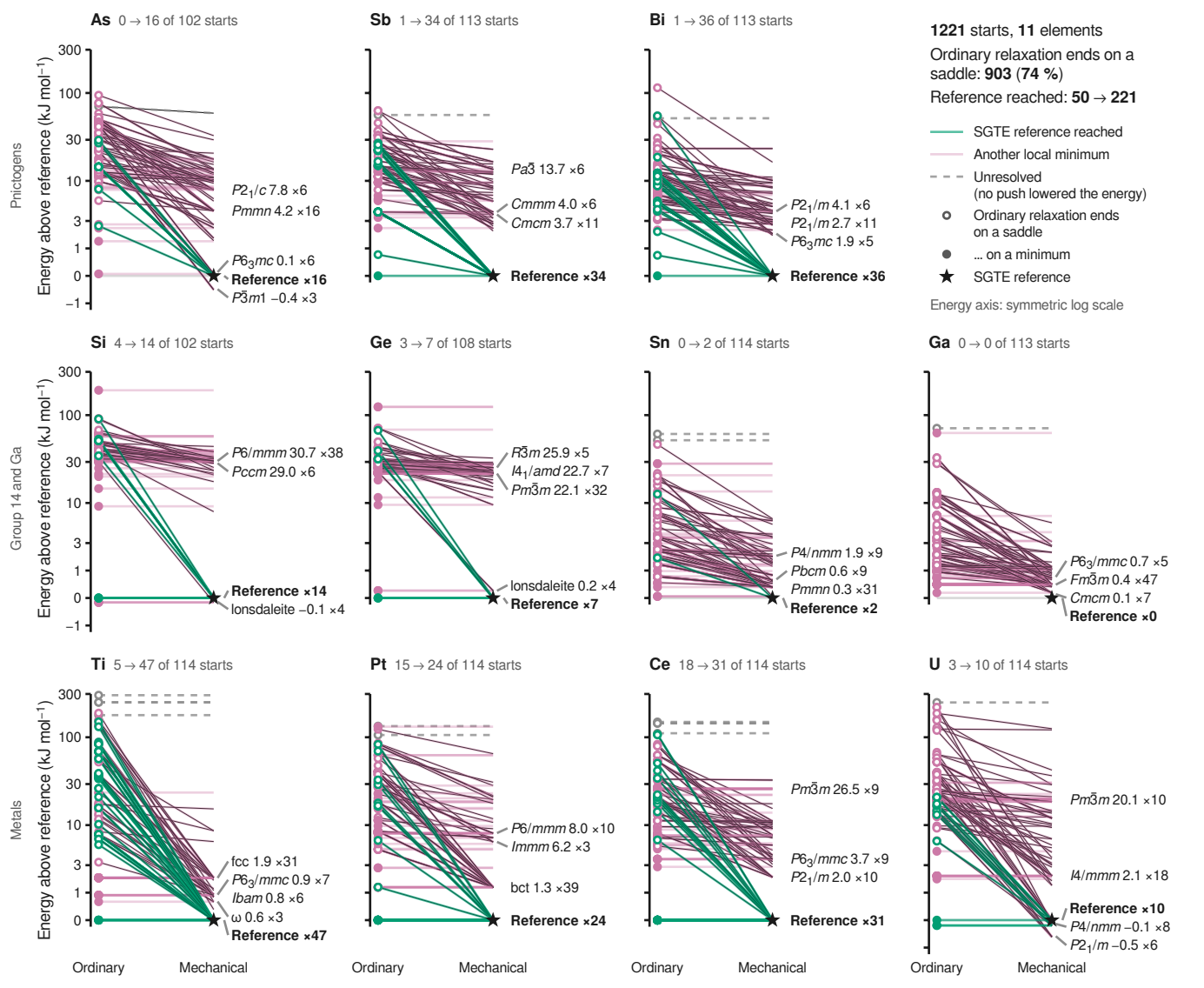
As 0 → 16 of 102 starts
Sb 1 → 34 of 113 starts
Bi 1 → 36 of 113 starts
1221 starts, 11 elements
Ordinary relaxation ends on a saddle: 903 (74 %)
Reference reached: 50 → 221
SGTE reference reached
Another local minimum
Unresolved (no push lowered the energy)
Ordinary relaxation ends on a saddle
... on a minimum
SGTE reference
Energy axis: symmetric log scale
Pnictogens
Group 14 and Ga
Metals
Energy above reference (kJ mol⁻¹)
300
100
30
10
3
1
0
−1
P2₁/c 7.8 ×6
Pmmn 4.2 ×16
P6₃mc 0.1 ×6
Reference ×16
P3̄m1 −0.4 ×3
Pa3̄ 13.7 ×6
Cmmm 4.0 ×6
Cmcm 3.7 ×11
Reference ×34
P2₁/m 4.1 ×6
P2₁/m 2.7 ×11
P6₃mc 1.9 ×5
Reference ×36
Si 4 → 14 of 102 starts
Ge 3 → 7 of 108 starts
Sn 0 → 2 of 114 starts
Ga 0 → 0 of 113 starts
P6/mmm 30.7 ×38
Pccm 29.0 ×6
Reference ×14
lonsdaleite −0.1 ×4
R3̄m 25.9 ×5
I4₁/amd 22.7 ×7
Pm3̄m 22.1 ×32
lonsdaleite 0.2 ×4
Reference ×7
P4/nmm 1.9 ×9
Pbcm 0.6 ×9
Pmmn 0.3 ×31
Reference ×2
P6₃/mmc 0.7 ×5
Fm3̄m 0.4 ×47
Cmcm 0.1 ×7
Reference ×0
Ti 5 → 47 of 114 starts
Pt 15 → 24 of 114 starts
Ce 18 → 31 of 114 starts
U 3 → 10 of 114 starts
fcc 1.9 ×31
P6₃/mmc 0.9 ×7
Ibam 0.8 ×6
ω 0.6 ×3
Reference ×47
P6/mmm 8.0 ×10
Immm 6.2 ×3
bct 1.3 ×39
Reference ×24
Pm3̄m 26.5 ×9
P6₃/mmc 3.7 ×9
P2₁/m 2.0 ×10
Reference ×31
Pm3̄m 20.1 ×10
I4/mmm 2.1 ×18
Reference ×10
P4/nmm −0.1 ×8
P2₁/m −0.5 ×6
Ordinary
Mechanical