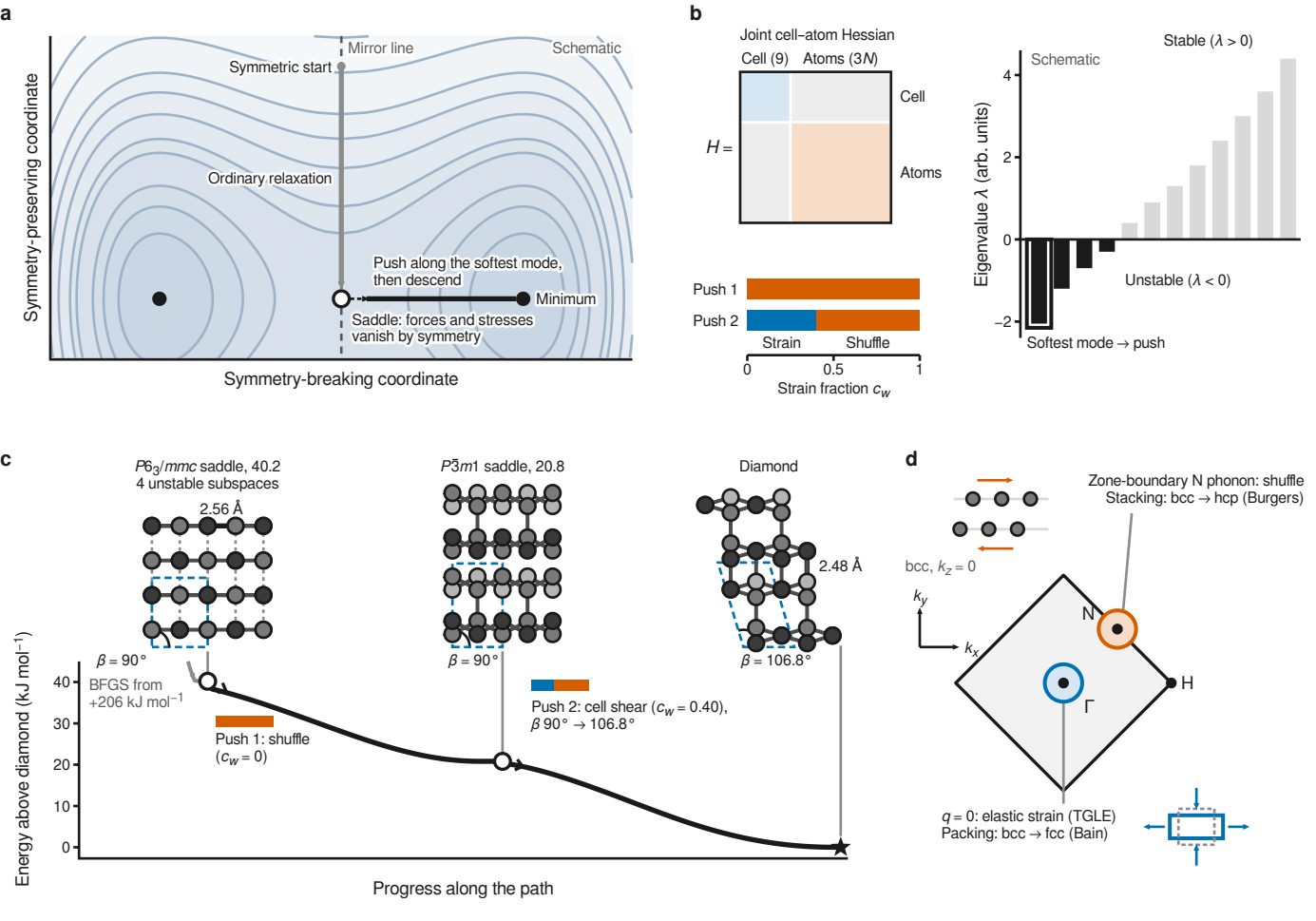
a
Symmetry-preserving coordinate
Symmetry-breaking coordinate
Mirror line
Schematic
Symmetric start
Ordinary relaxation
Push along the softest mode, then descend
Minimum
Saddle: forces and stresses vanish by symmetry
b
Joint cell–atom Hessian
Cell (9)
Atoms (3N)
H =
Cell
Atoms
Push 1
Push 2
Strain
Shuffle
0
0.5
1
Strain fraction c_w
Stable ($\lambda > 0$)
Schematic
Eigenvalue λ (arb. units)
4
2
0
−2
Unstable ($\lambda < 0$)
Softest mode → push
c
$P6_3/mmc$ saddle, 40.2
4 unstable subspaces
2.56 Å
$P\bar{3}m1$ saddle, 20.8
Diamond
2.48 Å
$\beta = 90°$
$\beta = 90°$
$\beta = 106.8°$
BFGS from +206 kJ mol^{-1}
Push 1: shuffle ($c_w = 0$)
Push 2: cell shear ($c_w = 0.40$), β 90° → 106.8°
Energy above diamond (kJ mol^{-1})
40
30
20
10
0
Progress along the path
d
bcc, $k_z = 0$
k_y
k_x
Zone-boundary N phonon: shuffle
Stacking: bcc → hcp (Burgers)
N
H
Γ
$q = 0$: elastic strain (TGLE)
Packing: bcc → fcc (Bain)