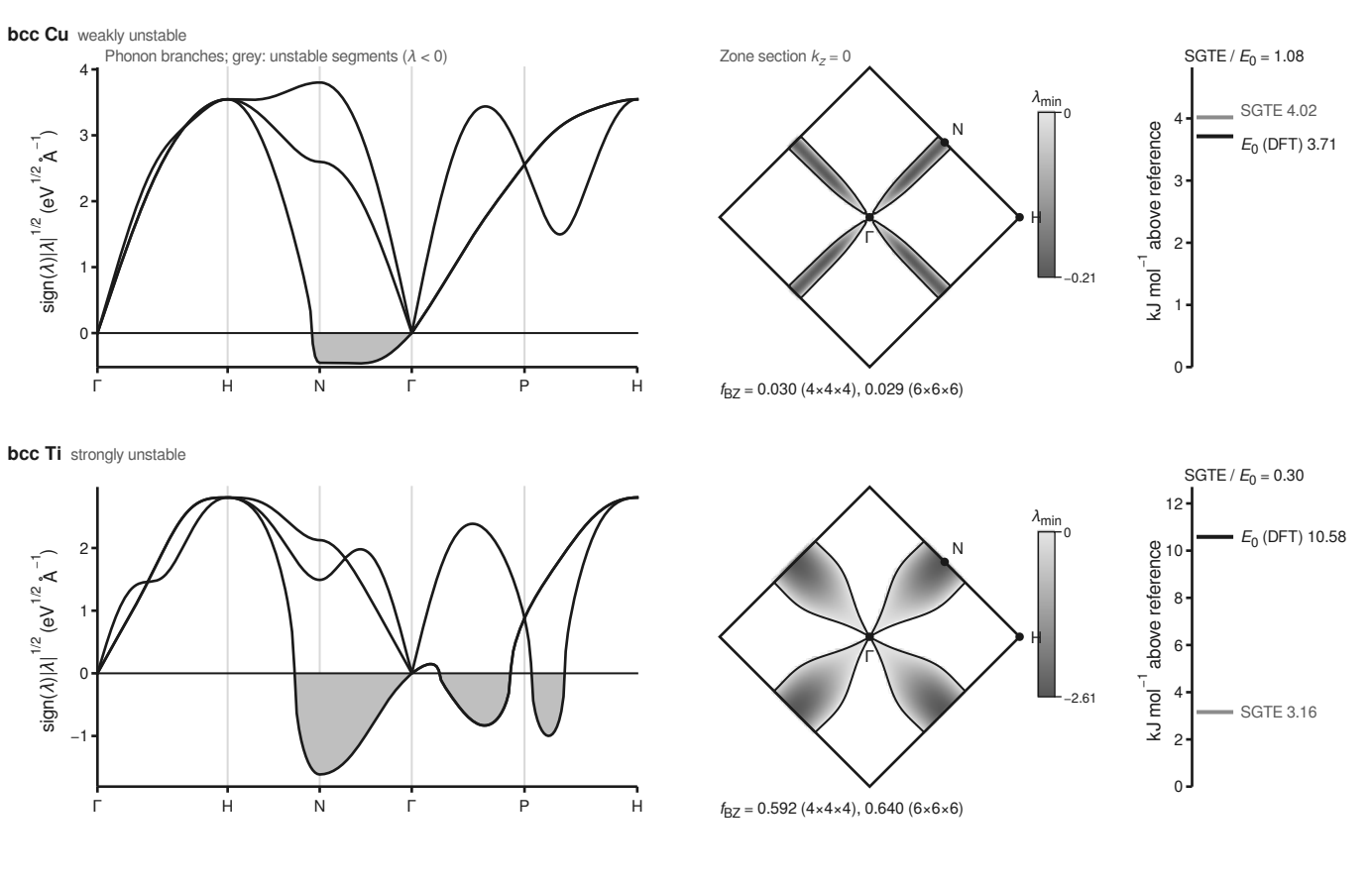
bcc Cu weakly unstable
Phonon branches; grey: unstable segments (λ < 0)
sign(λ)|λ|^1/2 (eV^1/2 Å^−1)
Γ H N Γ P H
Zone section k_z = 0
λ_min
0
−0.21
N
H
Γ
f_BZ = 0.030 (4×4×4), 0.029 (6×6×6)
SGTE / E_0 = 1.08
SGTE 4.02
E_0 (DFT) 3.71
kJ mol^−1 above reference
bcc Ti strongly unstable
sign(λ)|λ|^1/2 (eV^1/2 Å^−1)
Γ H N Γ P H
λ_min
0
−2.61
N
H
Γ
f_BZ = 0.592 (4×4×4), 0.640 (6×6×6)
SGTE / E_0 = 0.30
E_0 (DFT) 10.58
SGTE 3.16
kJ mol^−1 above reference