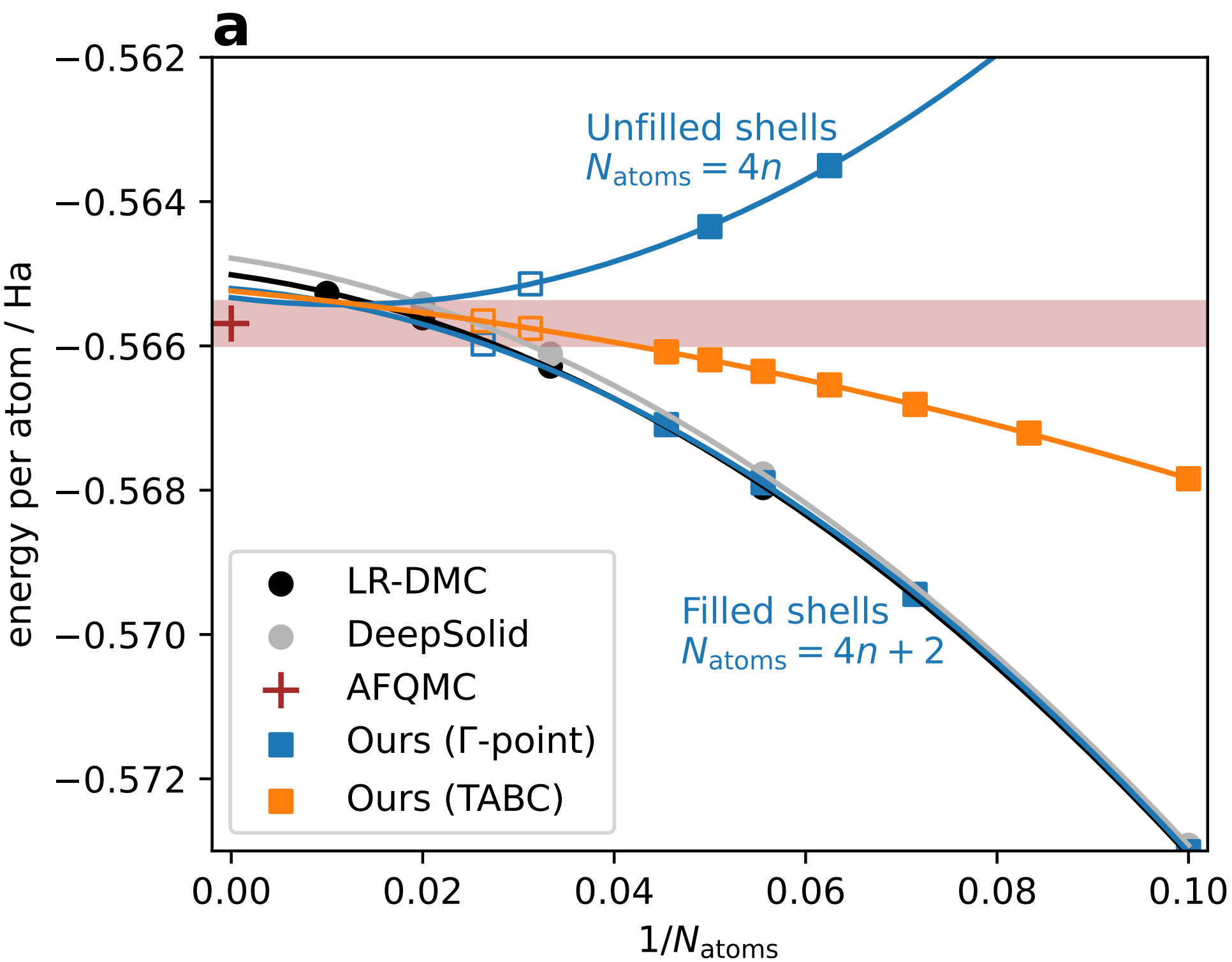
a
−0.562
−0.564
−0.566
−0.568
−0.570
−0.572
energy per atom / Ha
0.00
0.02
0.04
0.06
0.08
0.10
1/N_atoms
Unfilled shells
N_atoms = 4n
Filled shells
N_atoms = 4n + 2
LR-DMC
DeepSolid
AFQMC
Ours (Γ-point)
Ours (TABC)