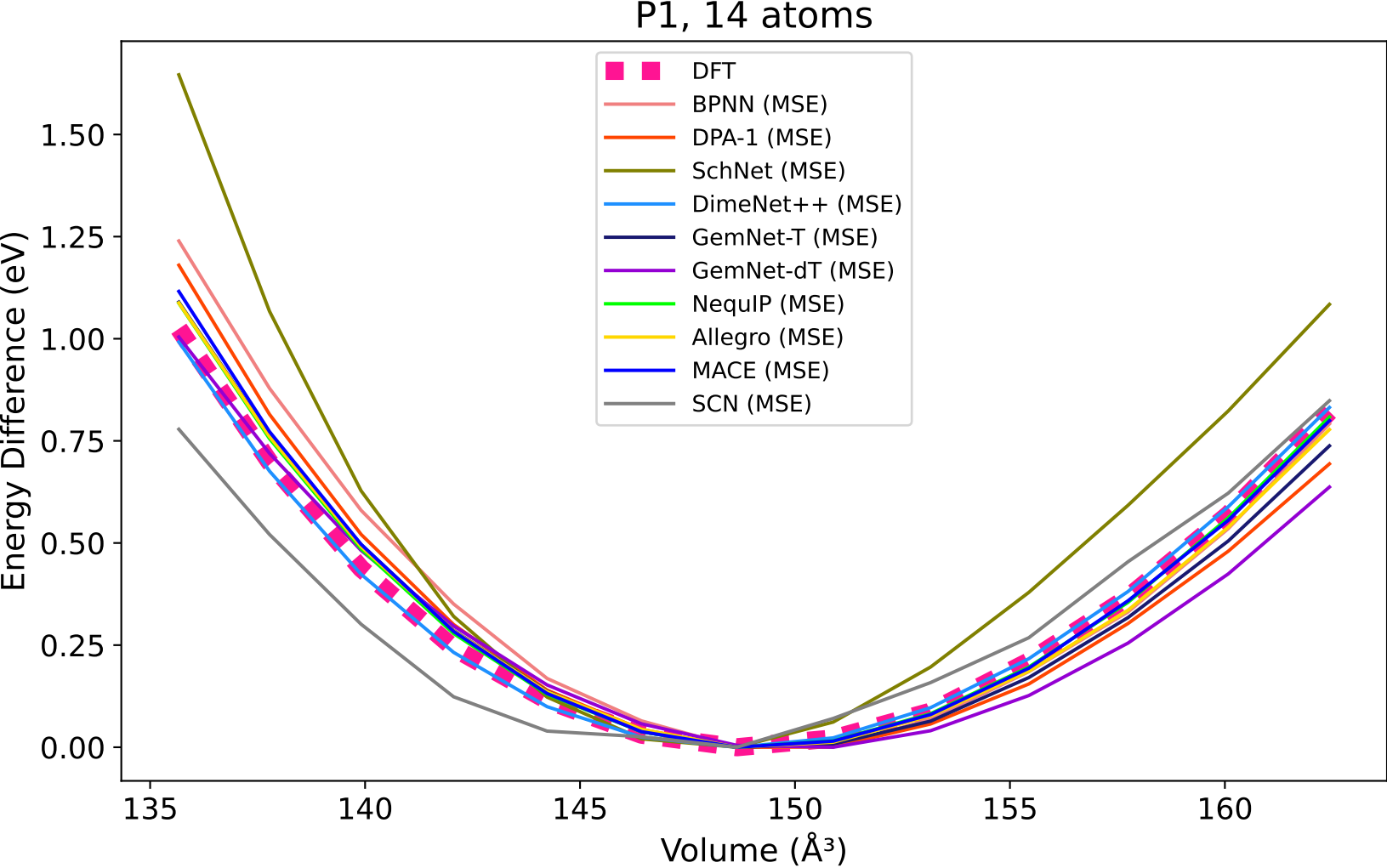
P1, 14 atoms
DFT
BPNN (MSE)
DPA-1 (MSE)
SchNet (MSE)
DimeNet++ (MSE)
GemNet-T (MSE)
GemNet-dT (MSE)
NequIP (MSE)
Allegro (MSE)
MACE (MSE)
SCN (MSE)
Energy Difference (eV)
1.50
1.25
1.00
0.75
0.50
0.25
0.00
135
140
145
150
155
160
Volume (Å³)