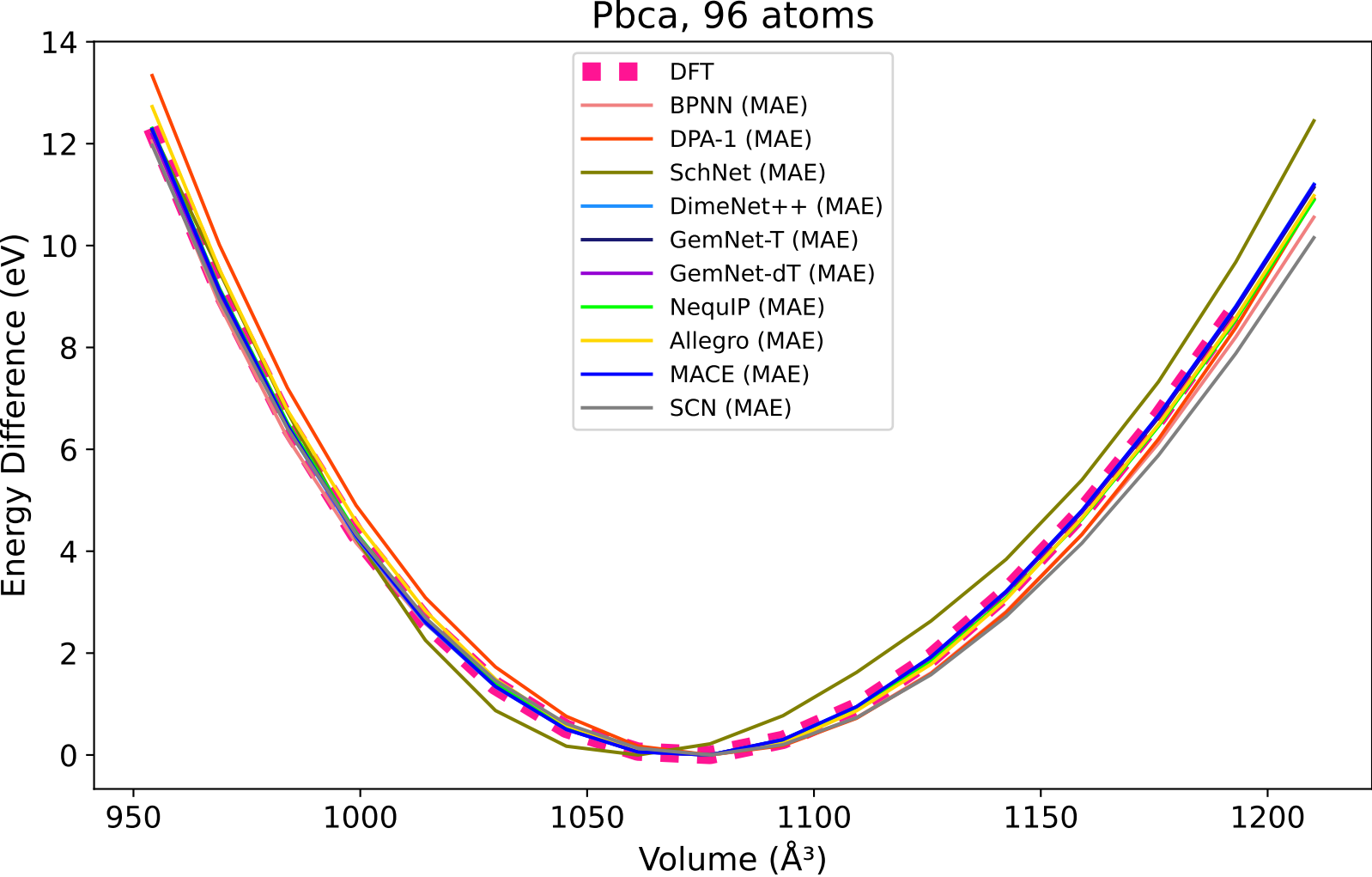
Pbca, 96 atoms
DFT
BPNN (MAE)
DPA-1 (MAE)
SchNet (MAE)
DimeNet++ (MAE)
GemNet-T (MAE)
GemNet-dT (MAE)
NequIP (MAE)
Allegro (MAE)
MACE (MAE)
SCN (MAE)
Energy Difference (eV)
Volume (Å³)
0
2
4
6
8
10
12
14
950
1000
1050
1100
1150
1200