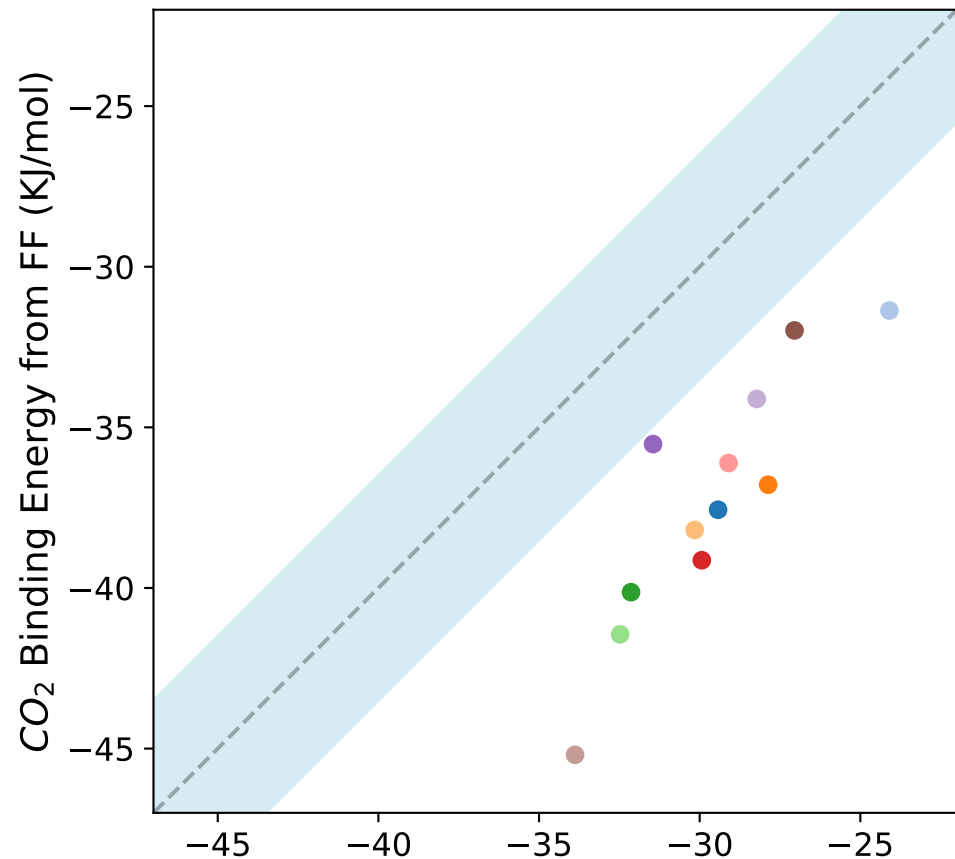
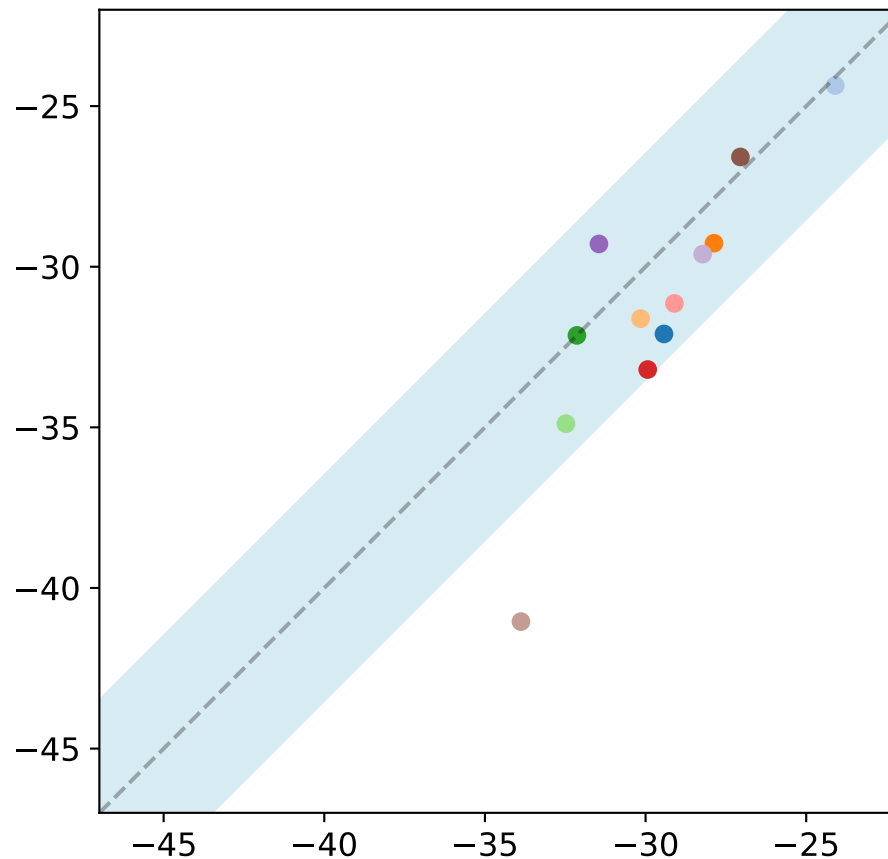


UFF

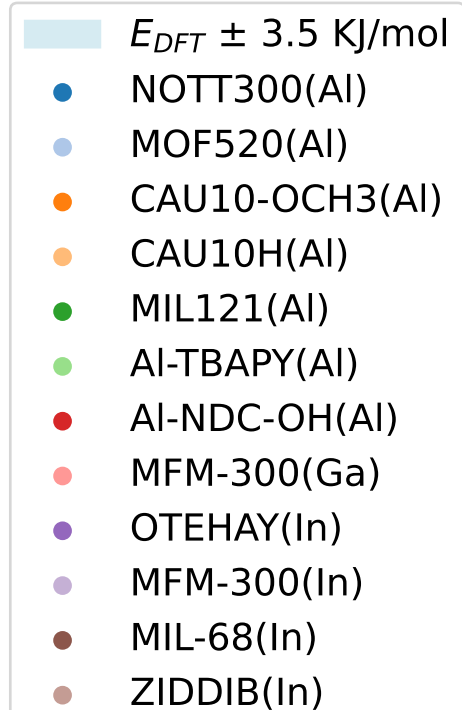


(a)

Refined FF



(b)



CO₂ Binding Energy from DFT-calculation (KJ/mol)