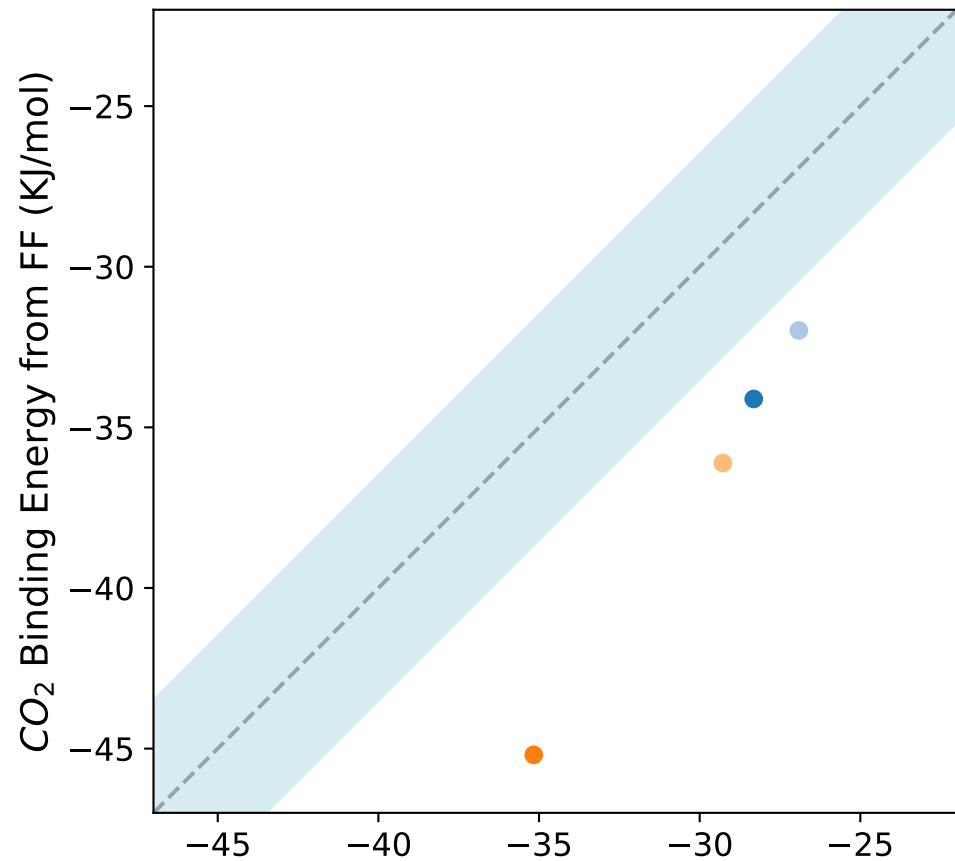
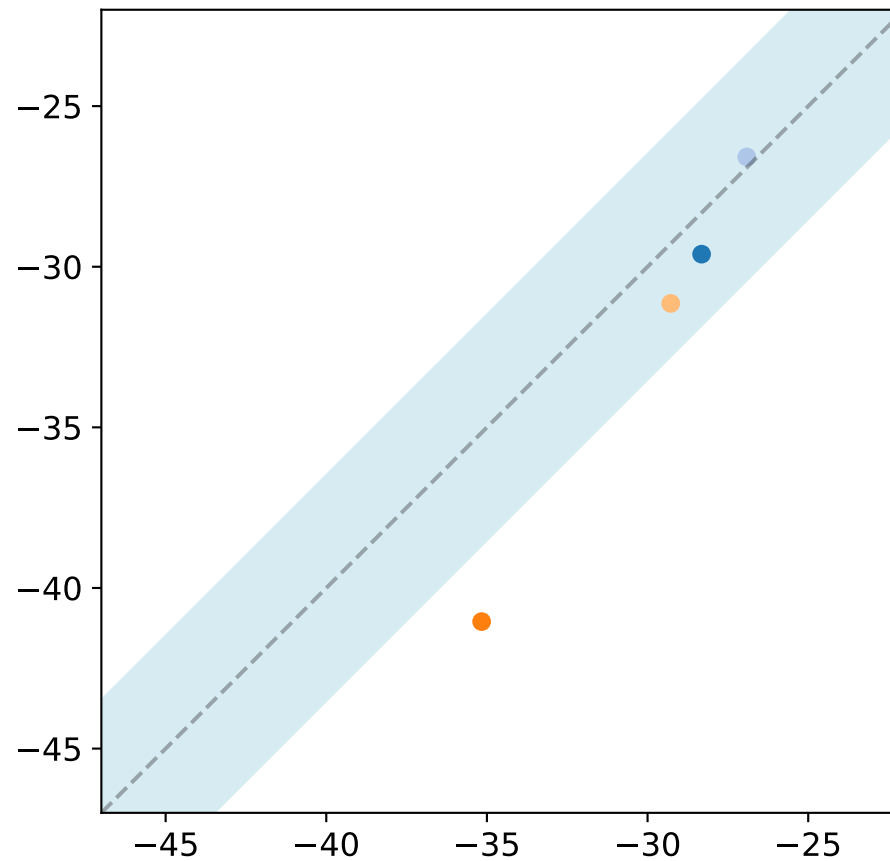


UFF



(a)

Refined FF



(b)

CO<sub>2</sub> Binding Energy from DFT-calculation (KJ/mol)