Adsorption isotherm of CO2 in silicic FAU

Dependency on the grid step size 10^{2} Average number of molecule per unit cell 10¹ - Reference GCMC Step size = 0.15 Å 10⁰ Step size = 0.2 Å Step size = 0.25 Å Step size = 0.3 Å 10^{-1} Step size = 0.35 Å Step size = 0.4 Å Step size = 0.45 Å 10⁻² -→ Step size = 0.5 Å 10^{2} 10^{4} 10⁶

Pressure (Pa)