

Atomistic investigation of functionalized silica pores for CO₂ capture

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Silica aerogels are highly amorphous materials characterized by a porosity that can reach 99 % and pore size distribution typically in the range of 2-50 nm. These characteristics result in a very low density (lower than 0.5 g/cm³) and a very high specific surface area (typically in the order of 1000 m²/g). The high porosity and specific surface area make aerogels suitable adsorbents, and their pore surface can be functionalized with different groups for selective adsorption of a particular gas, such as CO₂. By means of Molecular Dynamic (MD) simulations we investigate the adsorption mechanism of CO₂ molecules within single silica pores with different physico-chemical features. We study the influence of different physical properties (surface roughness, arrangement of functional groups) and chemical heterogeneity (type of surface groups) of the pore surface on their affinity for and mobility of CO₂. In particular, one of our key findings is that the surface defects, characterising the amorphous material (Fig. 1a) and not the crystalline (Fig. 1b), have an impact on its adsorption behaviour. Based on the simulation results, we extract the most relevant parameters that describe the adsorption at larger scale. We report the key findings of the atomistic investigation and discuss the relevant surface properties that need to be considered for a faithful upscaled description of the macroscopic flow and adsorption of CO₂ within porous silica. In particular, we focus on the differences between amorphous and crystalline substrates and we pinpoint the strengths and limitations of the employed force fields (Teter force field [1] for melt and quench of amorphous surfaces, and ClayFF [2], EPM2 [3] and CHARMM [4] combined to allow the description of different silica substrates, the CO₂ and the organic functionalization, respectively).

References

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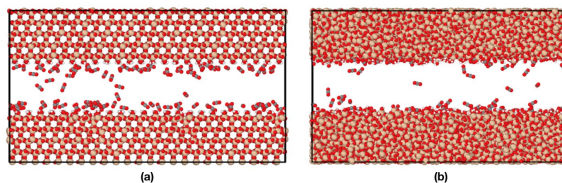


Fig. 1: Representation of CO₂ molecules absorption in a) crystalline and b) amorphous silica slit pore. Oxygen atoms in red, Silicon atoms in gold and Carbon atoms in grey.