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Improved understanding of adsorption and surface mobility of different gas in amorphous silica pores with different surface functional

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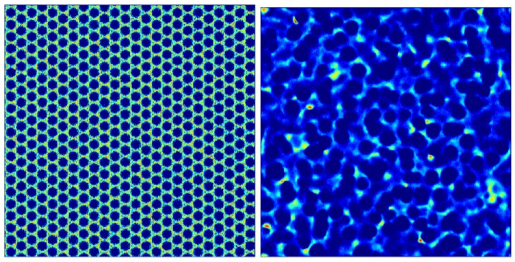
We investigate the adsorption mechanisms of CO_2 and CH_4 molecules in silica amorphous nanopores characterized by different physico-chemical features. We study the influence of different physical properties (e.g., local surface roughness) and chemical heterogeneity (e.g., number of hydroxyl, -OH, and ethoxyl (-OCH_2-CH_3) groups at the nanopore surface) on the affinity for CO_2 and CH_4, as well as on the resulting mobility. Hydroxyl and ethoxyl are among the most common surface groups found on silica substrates that are synthesized from the Tetraethyl orthosilicate (TEOS) precursor. Particular emphasis is placed on the effect of the amorphous surface features. Recently, we have demonstrated by Molecular Dynamics (MD) simulations the differences between the adsorption of CO_2 in crystalline (Fig 1a) and amorphous (Fig 1b) silica nanopores [1]. In
contrast to crystals, amorphous surfaces are characterized by a disordered structure that dictates adsorption at the surface. As a result, the adsorption patterns of the gas at the amorphous pore surfaces are irregular and difficult to characterize. In order to capture these features, we employ a segmentation algorithm to identify and extract the irregular adsorption patterns based on the average surface density of the sorbate; we then look at the mobility and residence time of gas molecules adsorbed at different classes of surface features. From an application point of view, the heterogeneous features of the amorphous nanosurfaces (e.g., roughness, functional groups, hydroxyl groups, oxygen vacancies) locally enhance CO_2 adsorption, potentially making amorphous material interesting for many industrial applications (including catalytic processes [2]). A recent work [3] showed the potential of hydrophilic (high density of -OH groups) and hydrophobic (high density of -OCH_2-CH_3) membranes for fluid separation.



(a) (b)

Figure 1: CO_2 density maps: regular patterns at the crystalline surface (a), irregular patterns at the amorphous surface (b).

References

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