Assessing CO_2 Capture in Porous Sorbents via ssNMR-Assisted Adsorption Techniques

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Our group has recently explored solid-state (ss) NMR methodologies to collect adsorption data, profiting from the numerous advantages offered by standard high-resolution ssNMR techniques, such as high-field magnet and Magic-Angle-Spinning (MAS). These features are crucial for recording comprehensive adsorption isotherms of confined non-protonated gas molecules, such as CO_2. This work gathers all methodologies developed in our previous studies, wherein we applied variable pressure ssNMR for assessing CO_2 adsorption mechanisms on mesoporous silicas. Altogether, these ssNMR methodologies allow the acquisition of CO_2 adsorption isotherms enabling the identification and quantification of distinct chemisorbed and physisorbed CO_2 species.

Figure 1 contains a schematic illustration of the various methodologies applied to record full gas adsorption isotherms, using $^{13}CO_2$ adsorbed on amine-modified mesoporous silicas (APTES@SBA-15). Our approach, has the advantage to differentiate between physisorbed and chemisorbed CO_2 fractions, allowing the identification of six distinct types of confined CO_2 species. This work represents a major contribution to the adsorption research community, as traditional techniques like volumetric or gravimetric adsorption can not distinguish between different CO_2 species. Moreover, it seamlessly integrates spectroscopic and gas adsorption measurements, enabling a comprehensive characterization of the CO_2 adsorption processes in porous materials at the molecular scale. Our group is currently applying this methodology to a wider range of materials, including zeolites, porous carbons, covalent organic frameworks (COFs) and metal-organic frameworks (MOFs), demonstrating its potential to obtain deeper structural insight into gas adsorption mechanisms and separation processes, which will ultimately contribute towards the development of improved solid adsorbents.

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FIGURE 1
Schematics describing the methodology used to perform qualitative and quantitative characterization of different chemi- (A, B and C) and physisorbed (D, E and F) CO_2 species formed at different gas partial pressures in APTES@SBA15.