Poster

In situ PXRD studies of poly(heptazine imide)-based adsorbents

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Despite numerous studies on post-combustion CO_2 capture the search for efficient adsorbents continues. Alternative to conventionally applied sorbents can be found in polymeric carbon nitride class of materials, also known as poly(heptazine imides) (PHIs). PHI possesses the following advantages: chemical and thermal stability, easy to scale up, precursors are abundant and inexpensive yielding an economic final product. So far it has mainly attracted attention as (photo)catalyst for hydrogen, hydrogen peroxide production, CO_2 and biomass conversion. Works reporting CO_2 adsorption on carbon nitrides are scarce. The common feature of these studies is the amorphous state of the material sometimes on the border of being disordered N-doped carbons. Therefore, the interest towards a crystalline, well-structured PHI has arisen. Recently Burrow et al. [1] reported the performance of crystalline CaPHI in CO_2 adsorption. They were able to synthesize a microporous PHI sorbent with the promising CO_2 capture capacity. In this work we have developed adsorbents based on PHI in its sodium form. The prepared adsorbents are able to selectively adsorb CO_2 with high capacities. We attribute this efficient performance to the effect of stacking of layers that form microporous channels able to capture CO_2 molecules. Additionally, in-situ PXRD studies have demonstrated that the temperature regime of the material pre-treatment and adsorption affects to great extent the structural features of the sorbent and it is of crucial importance for the CO_2 uptake by PHIs.

[1] Burrow, J., Ciufo, R., Smith, L., Wang, Y., Calabro, D., Henkelman, G., Mullins, B. (2022) *ACS Nano* **16**, 5393.

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