## Influence of PANI loading in hierarchically porous PANI/ZIF-8 composites on their sorption properties

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In the fight for reducing the carbon dioxide (CO<sub>2</sub>) emissions, carbon capture technologies are a powerful tool. There, the adsorption onto porous sorbents is recently gaining interest as a promising alternative to conventional sour gas removal by absorption into ionic liquids, a well established, yet energetically very demanding process. The quest is for highly effective and selective CO<sub>2</sub> sorbents, disposing of high reversible adsorption capacity coupled with maximal affinity to CO<sub>2</sub>. A variety of compounds are therefore being investigated for the key properties indicating a high potential for applicability in the CO<sub>2</sub> adsorption field.

Zeolitic imidazolate frameworks (ZIFs) are, for their high specific surface area, porous structure, surface functionality and thermo-chemical robustness, one of the leading candidate materials. This work exploits the potential of the ZIF-8 compound, focusing on its high-yield preparation while reproducing the previously reported CO<sub>2</sub> sorption properties. It further aims to improve the ZIF-8 adsorption performance by doping with a nitrogen-rich polymer, polyaniline (PANI).

Five different PANI/ZIF-8 composites with different PANI loadings (15%, 30%, 40%, 60% and 80%) were prepared and studied by a combination of characterization techniques, including FTIR, SEM and TEM. Five hierarchically porous carbon adsorbents were derived via thermal and chemical co-activation by KOH from the prepared composites, introducing hierarchical porosity into the material, to promote efficient diffusion and adsorption of the CO<sub>2</sub> gas. It was found that the combination of these steps, solely, improved the CO<sub>2</sub> capacity by 280% compared to original materials.

Furthermore, the impact of PANI loading in the hierarchically porous adsorbent materials on their sorption properties, such as specific surface area, micropore volume and CO<sub>2</sub> uptake, was studied. The best performing materials, in terms of CO<sub>2</sub> capacity, showed a 60% and 15% increase in amount of CO<sub>2</sub> adsorbed, compared to carbons derived from building block materials, ZIF-8 and PANI, respectively, reaching sorption capacity of 6.3 mmol/g at 1 bar. A correlation between micropore volume and CO<sub>2</sub> capacity of the adsorbents was proven, peaking at PANI loadings between 40% and 80%.

Finally, a durability test performed upon the best hierarchically porous composites revealed an excellent ability to regenerate of these materials, at low energy consumption conditions.

Keywords: zeolitic imidazolate frameworks, ZIF-8, porous adsorbents, CO<sub>2</sub> capture.

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