Rational design and synthesis of covalent triazine frameworks based on novel N-heteroaromatic building blocks for efficient CO_2 and H_2 capture and storage

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Covalent Triazine Frameworks (CTFs), a nitrogen-rich subclass of Porous Organic Polymers (POPs), show large potential in applications including gas adsorption /separation and heterogeneous catalysis due to their distinctive large surface area, low skeleton density, good thermal and chemical stability combined with their rational tunability.[1] Herein, we reported on a set of nitrogen-rich CTFs prepared by trimerization of 4,4',4'',4'''-(1,4-phenylenebis(pyridine-4,2,6-triyl))tetrabenzonitrile under ionothermal conditions. The influence of several parameters such as $ZnCl_2$/monomer ratio and reaction temperature on the structure and porosity of the resulting frameworks was systematically examined. After a thorough characterization, their performance in CO_2 and H_2 adsorption as well as their selectivity of CO_2 over N_2 was assessed. Notably, the CTF obtained using 20 molar equiv. of $ZnCl_2$ at a reaction temperature of 400 °C exhibits an excellent CO_2 adsorption capacity (3.48 mmol/g at 273 K and 1 bar) as well as a significant high H_2 uptake (1.5 wt% at 77 K and 1 bar). These values are among the highest measured under identical conditions to date. In addition, the obtained CTFs also present a relatively high CO_2/N_2 selectivity (up to 36 at 298 K) making them promising adsorbents for gas sorption and separation.

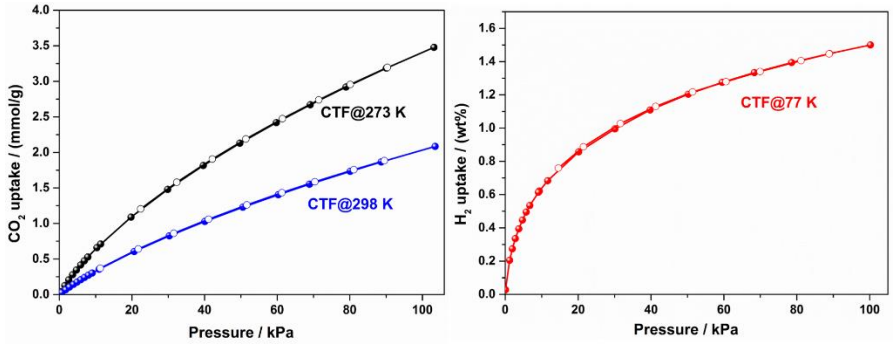

Figure 1. CO_2 (left) and H_2 (right) adsorption isotherms of the obtained CTF synthesized at 400 degrees and 20 molar equivalents of $ZnCl_2$.

Reference

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