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

Guang-Bo Wang,$^1$ Karen Leus,$^1$ Shu-Na Zhao,$^1$ Ying-Ya Liu$^2$ and Pascal Van Der Voort$^{1*}$

$^1$ Ghent University, Department of Inorganic and Physical Chemistry, Center for Ordered Materials, Organometallics and Catalysis (COMOC); Krijgslaan 281 (S3), 9000 Ghent, Belgium.
$^2$ State Key Laboratory of Fine Chemicals, Dalian University of Technology, 116024 Dalian, People’s Republic of China.

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


Website: [www.comoc.ugent.be](http://www.comoc.ugent.be); Email: guangbo.wang@ugent.be