Functionazation of MOFs via Solvent-Assisted Ligand Incorporation (SALI) for CO₂ Capture

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Introduction

Incorporation of desired functionality into MOFs is often problematic during de novo synthesis. However, post synthesis incorporation is a key strategy. Herein we report a new functionalization technique, solvent assisted ligand incorporation (SALI), to efficiently incorporate carboxylate-based functionalities in the Zr-based metal-organic framework, NU-1000. SALI introduces functional groups as charge compensating and strongly bound moieties to the Zr₆ node. Utilizing SALI, we have efficiently attached perfluoroalkane-carboxylates of various chain lengths (C₆-C₈) on the Zr₆ nodes of NU-1000. These fluoroalkane-functionalized mesoporous MOFs, termed herein, SALI-n were studied experimentally and theoretically as potential CO₂ capture materials.

Results

PXRD, DRIFTS and N₂ Isotherms of SALI-n

- PXRD revealed that SALI-n maintain their crystallinity after SALI.
- DRIFTS data indicate that new carboxylate group incorporation occurs via replacing the terminal hydroxyl groups.
- Increasing perfluoroalkyl chain reduces pore volume and surface area.

SALI-7: Modeling of CO₂ adsorption

- We have developed an efficient functionalization method for Zr-based mesoporous MOFs based on solvent assisted ligand incorporation (SALI).
- Spectroscopic data indicate that these carboxylates are bound to the Zr₆ node, likely resulting in a UiO-66 type metal node, Zr₆[(µ₂-OH)₆][(µ₂-OR)₆}(R(CO₂))₁₂.
- CO₂ adsorption studies indicate that perfluoroalkane-functionalized nodes in the SALI-n system synergistically act as the primary CO₂ binding sites manifesting in systematically higher values for Q₈, with increasing in chain length.

Conclusions

Acknowledgements

References