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The roles of functional carbonyl-based materials in energy storage and gas separations

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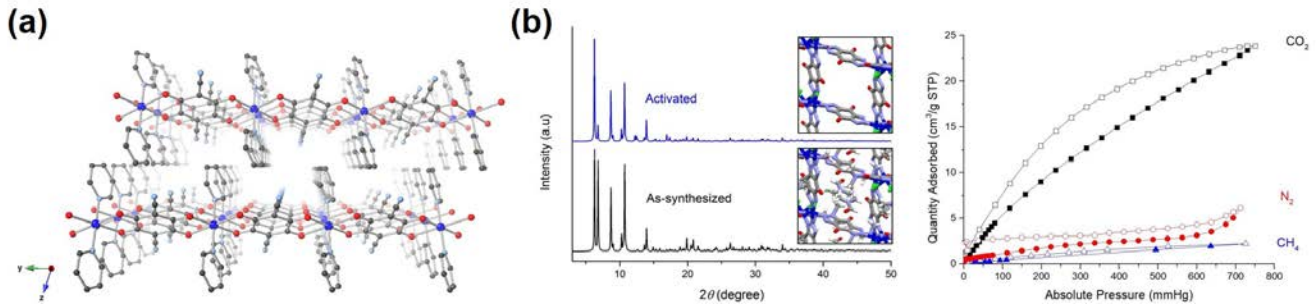
Abstract

A series of carbonyl-containing molecules were used as organic building blocks for coordination polymers (CPs), metal–organic frameworks (MOFs), and porous molecular crystals (PMCs). We synthesized a novel ligand 1,4-dicyano-2,3,5,6-tetrahydroxybenzene (LH_4), and the resulting redox-active 1D copper-benzoquinoid CPs $[CuL(DMF)_2]_n$ and $[CuL(Py)_2]_n$ were used as cathode materials for lithium-ion batteries (Figure a).[1] $[CuL(DMF)_2]_n$ is able to deliver an initial capacity as high as 268 mA h g^{-1} at 30 mA g^{-1}. Electrode composed of $[CuL(Py)_2]_n$ gives an ultrahigh power density over 13,000 W kg^{-1}. The structure-property relationships of these crystalline materials are studied through the synchrotron powder X-ray diffraction (PXRD). The obtained mechanistic understanding of the metal–organic electrode materials for Li-based batteries may pave the way for the design of next-generation energy-storage systems.

In addition, porous materials incorporated with polar carbonyl groups can provide a unique platform for host-guest interactions, which lead to superior molecular separation performance. We have prepared a MOF built from quinone-cored bis(triazole) ligand and Cu(II) (Figure b). This material exhibits the ability to capture CO_2 but negligible N_2 adsorption at 298K. The changes of synchrotron PXRD patterns upon the adsorption of various gases prove the unique interactions between the guest molecules and frameworks. Accordingly, the carbonyl-based porous materials are very promising for the applications on gas separations.



Keywords – Metal-organic materials, porous materials, gas separations, energy storage.

Reference

[1] C.-H. Chang, A.-C. Li, I. Popovs, W. Kaveevivitchai, J. L. Chen, K.-C. Chou, T.-S. Kuo, T.-H. Chen, "Elucidating metal and ligand redox activities of copper-benzoquinoid coordination polymer as cathode for lithium-ion batteries," *J. Mater. Chem. A*, 2019, vol. 7, pp. 23770-23774.