



Review

Porous metal–organic frameworks for fuel storage

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ABSTRACT

Methane and acetylene represent cleaner fuels, which are considered as ideal alternatives to fossil fuels. Due to low volumetric energy density at ambient conditions, it is highly desirable to develop porous materials such as metal–organic frameworks that exhibit good adsorption properties with respect to them. In this review, we firstly introduced the development history on the design and synthesis of porous metal–organic frameworks for acetylene and methane storage in which some representative examples were analyzed; and then we focused on discussing their adsorption mechanisms including the gas binding sites and gas–framework interactions. At last, some structure–property relationships and synthetic strategies for improving gas adsorption properties with respect to them were summarized.

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Abbreviations: adc, 9,10-anthracenedicarboxylate; ANG, adsorbent natural gas; bdp, 1,4-benzenedipyrzolate; 4,4'-bpy, 4,4'-bipyridine; BTAC, benzene-1,3,5-β-acrylate; BTB, benzene-1,3,5-tribenzoate; BET, Brunauer–Emmett–Teller; bdc, 1,4-benzenedicarboxylate; BPDC, biphenyldicarboxylate; dabco, 1,4-diazabicyclo[2.2.2]octane; DFT, density functional theory; DHTP, 2,5-dihydroxyterephthalate; DMA, *N,N*-dimethylacetamide; DMF, *N,N*-dimethylformamide; DOE, Department of Energy; GCMC, grand canonical Monte Carlo; H₂btc, 1,3,5-benzenetricarboxylic acid; HCPT, 4-(4-carboxyphenyl)-1,2,4-triazole; HETCOR, heteronuclear chemical shift correlation; Hetz, 3,5-diethyl-1,2,4-triazole; HINA/jna, isonicotinic acid; Hpypz, 4-(1H-pyrazol-4-yl)pyridine; H₂TZB, 4-(1H-tetrazol-5-yl)benzoic acid; IRMOF, isoreticular metal organic framework; MBB, molecular building block; MeIM, 2-methylimidazole; MEM, maximum entropy method; MFM, Manchester Framework Material; MIL, Matériaux de l'Institut Lavoisier; MOF, metal organic framework; MTV-MOF, multivariate metal organic framework; ndc, 1,4-naphthalenedicarboxylate; NGV, Natural Gas Vehicles; NMR, nuclear magnetic resonance; *pacs*, partitioned acs; PCN, porous coordination network; pia, *N*-(pyridin-4-yl)isonicotinamide; PSP, pore space partition; pyz, pyrazine; pzdc, pyrazine-2,3-dicarboxylate; SBU, secondary building unit; STP, standard temperature and pressure; TED/ted, triethylenediamine; TCDPA, 3',3'',5',5''-tetrakis(4-carboxyphenyl)-9,10-diphenylanthracene; TCDPN, 3',3'',5',5''-tetrakis(4-carboxyphenyl)-1,4-diphenylanthracene; TCPT, 3',3'',5',5''-tetrakis(4-carboxyphenyl)-*p*-terphenyl; TPDC, terphenyldicarboxylate; TPT/tpt, 2,4,6-tri(4-pyridinyl)-1,3,5-triazine; vdW, van der Waals; ZIF, zeolitic imidazolate framework.

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1. Introduction

The growing shortage of fossil fuels, combined with increasingly serious environmental issues and climate changes caused by the excessive carbon dioxide emission produced by burning fossil fuels, as a result of rapid industrialization and civilization, has spurred an initiative to develop alternative cleaner fuels. Among the various possible fuels, hydrogen is being considered as the most ideal clean energy source carrier because of its pollution-free burning and high chemical energy. In addition to hydrogen, natural gas, whose main component is methane, is also regarded as a preferable alternative fuel because of its potential for reduced carbon emission and higher thermal efficiency, coupled with the increasing accessibility. However, the volumetric energy density of hydrogen and methane under ambient conditions is relatively low, which severely hinders their widespread usage, in particular for mobile/transportation applications. Compression and liquefaction have been proposed to increase their volumetric energy density, which however suffer from high storage costs and safety issues resulting from the harsh operating conditions. As an alternative, adsorption technology using porous materials that bind gas molecules *via* van der Waals (vdW) interactions may offer an appealing option. The key to the success of adsorption technology lies in development of highly efficient porous materials that can store a large amount of gases at mild conditions.

To direct the research and development of porous materials for the above applications, the U.S. Department of Energy (DOE) has set up the targets for on-board hydrogen and methane storage. For hydrogen storage, the 2017 uptake targets are 5.5 wt% on a gravimetric basis, and 40 g L⁻¹ on a volumetric basis at an operating temperature of 233–333 K under a maximum pressure of 101 bar (ultimate targets: 7.5 wt% and 70 g L⁻¹) [1]. For methane storage, the U.S. DOE in 2000 set a storage target of 180 cm³ (STP) cm⁻³ (the volume of gas adsorbed at standard temperature and pressure *per* volume of the storage vessel) deliverable for an operational ANG (adsorbed natural gas) vehicular system working at a pressure of 35 bar and 298 K. Recently, the Advance Research Projects Agency-Energy (ARPA-E) of U.S. DOE updated the target for methane storage materials for ANG applications. Specifically, the adsorbent-level volumetric energy density at room temperature must be more than the energy density of CNG (compressed natural gas) at 298 K and 250 bar (9.2 MJ L⁻¹) which is equivalent to 263 cm³ (STP) cm⁻³. If the packing loss (25%) is taken into account, the adsorbent-level volumetric energy density must exceed 12.5 MJ L⁻¹ at room temperature, which corresponds to a volumetric storage capacity of 350 cm³ (STP) cm⁻³ for the adsorbent material. Additionally, to avoid a heavy tank, U.S. DOE also set a target concerning the gravimetric energy density of 0.5 g g⁻¹. These targets provide intuitive and useful guidance for the researchers working on adsorbent-based hydrogen and methane storage.

Besides hydrogen and methane, acetylene, as the simplest alkyne and unsaturated hydrocarbon, also plays a very important role in daily life and modern chemical industry. It is widely used as gas fuel for oxy-acetylene welding and metal cutting due to high oxy-acetylene flame temperature up to 3273–4273 K. Also, acetylene is utilized as a key starting material to manufacture various fine chemicals (such as vinyl chloride, and methyl acrylate) and

electronic materials. For its widespread use, one issue we have to address is concerning its storage which is very challenging because it cannot be stored in a steel cylinder under high pressure like hydrogen and methane due to its highly explosive nature. It is well known that pure acetylene stored at a pressure above 2 bar risks exploding at room temperature, even in the absence of oxygen. The current storage method involves dissolving acetylene in acetone placed in a vessel along with an adsorbent. Nevertheless, such a method suffers from low acetylene purity due to the volatile solvent contamination. Analogously, physical adsorption technology is regarded as one of the most competitive methods because of low cost and high efficiency, and is expected to overcome the above-mentioned issues. Therefore, development of new porous materials exhibiting high-capacity acetylene storage under ambient conditions is also highly desirable.

Emerging as a new class of porous materials, metal–organic frameworks (MOFs) have been investigated intensively over the past two decades and continue to receive considerable scientific interest. They are composed of metal ions or metal-containing clusters coordinated to polytypic organic bridged ligands to form multidimensional network structures having well-defined pore systems (channels, cages, *etc.*). Compared with the traditional activated carbons and zeolites, MOFs possess distinctive characteristics including large surface area, high porosity, chemically adjustable pore dimension and functionalized pore surface. Also, MOFs tend to possess the ordered crystal structures than can be determined by single-crystal X-ray diffractions, which is conducive to their structure–property relationship elucidations and functional optimizations. These attractive characteristics offer MOFs great promise for a wide variety of applications including but not limited to gas storage [1], molecule separation [2–14], heterogeneous catalysis [15–21], chemical sensing [22–24], and drug delivery [25]. In particular, porous MOFs are recognized as prospective adsorbents that can provide potential solutions to the enduring challenges pertaining to the safe storage and efficient use of hydrogen, methane and acetylene [6,26–32]. For hydrogen storage, the reader can refer to many excellent reviews [33–38]. Herein, we only discuss the current status related to acetylene and methane storage in porous MOFs.

2. Acetylene storage in MOFs

2.1. Design and synthesis of MOFs for acetylene adsorption: A brief history

Cu₂(pzdc)₂(pyz) is the first MOF whose acetylene adsorption properties were examined [39]. In the as-synthesized compound, the guest water molecules residing in one-dimensional (1D) channel interact *via* hydrogen bonding with the uncoordinated carboxylate oxygen atoms on the pore surface, indicating that these oxygen atoms on pore surface can potentially serve as active functional sites for binding guest molecules, especially those with acidic hydrogen atoms such as acetylene. These observations prompted the authors to investigate its acetylene adsorption properties (Fig. 1a). As they expected, the compound exhibited high adsorption affinity toward acetylene molecule (42.5 kJ mol⁻¹) with

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