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Dynamic Gas Separation on a Flexible Single-Crystal Host. Satoshi Takamizawa^{a,b}. ^aGraduate School of Nanobioscience, Yokohama City University. ^bJST-PRESTO

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Microporous materials, which have pores with diameters less than 20 Å, are attractive in both industry and scientific fields since they are applicable for gas separation, gas adsorption, and catalysis. I previously reported a porous single crystal of a metal complex $[\text{Cu}_2(\text{bza})_4(\text{pyz})]_n$ **1**, which has structural flexibility as well as regularity. The single crystal **1** easily adsorbed various gases through narrow channels with a diameter of ca. 2-4 Å.

While the design of sorption selectivity in porosity is mostly based on pore structure and adsorption interaction, flexibility can enable tuning the adsorption state by adjusting the host structure. To develop the dynamic gas selectivity, three kinds of separation for various organic vapors and inorganic gases were carried out for **1**: (1) chromatography on a microcrystal packed column,¹ (2) sorption from a vapor mixture,² and (3) permeation through single crystal of for various organic vapors and inorganic gases.³ The analyses of these results demonstrated the novel dynamic separation on flexible porous solid: (1) strong entropy dependence,¹ (2) dynamic switch of gas selectivity,² and (3) smooth and high selective permeation through narrow channels.³

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Structure and topology of novel zeolites and mesoporous materials. Junliang Sun^a, Charlotte Bonneau^a, Daliang Zhang^a, Yu Han^b, Corma Avelino^c, Xiaodong Zou^a. ^a*Inorganic and structural chemistry, Berzelii Center EXSELENT on Porous Materials, Stockholm University, Sweden.* ^b*King Abdullah University of Science and Technology, Saudi Arabia.* ^c*Instituto de Tecnología Química, Spain.*

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In the formation of mesoporous silica materials with surfactants, the interaction between inorganic species and surfactants plays a crucial role. The mesoporous materials commonly form a kind of interface which minimises the surface energy. It is quite often to see the silica wall follows so-called bi-continuous minimum surfaces, while no real example was found to present a tri-continuous minimum surface although it was predicted mathematically. IBN-9 is the first example which shows a tri-continuous pore structure with etc-c3 topology, and its silica wall follows a tri-continuous H-minimum surface.[1] IBN-9 was synthesized with a designed surfactant which enables the fine-tuning of the interface curvature. MCM-41-type and MCM-48-type mesostructures can also be synthesized with the same surfactant. The whole

system shows a good example of synthesizing mesostructures by controlling the interface curvature.

The minimum surfaces also appear in crystalline inorganic phases, especially for those with extra large pores, such as the germanate SU-M.[2] ITQ-37, a germanosilicate zeolite, is another example with its pore-size approaching the meso-scale.[3] Its structure was determined by a new approach: combining selected area electron diffraction (SAED) and powder X-ray diffraction (PXRD) in a charge-flipping algorithm. The framework of ITQ-37 follows the srs minimal net and its extra-large 30-rings form two unique cavities where each cavity is connected to three others to form a gyroidal channel system. These cavities describe the enantiomorphous srs net of the framework. Different from all known MCM-48-type mesostructures and other microporous structures, ITQ-37 is the first chiral zeolite with one single gyroidal channel and this channel is roughly separated from the framework by a G-minimum surface. It has the lowest framework density (10.3 T atoms per 1000 Å³) of existing 4-coordinated crystalline oxide frameworks, and the pore volume of the corresponding silica polymorph would be 0.38 cc.g⁻¹.

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Guest Ordering Inside MOF's Channels: Breathing Effect versus Steric Factors. Kirill Yussenko, Mikhail Meilikhov, Roland A. Fischer. *Inorganic Chemistry II, Ruhr-University Bochum, Germany.*

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The Porous Coordination Polymers (PCPs) or Metal-Organic Frameworks (MOFs) are a unique class of hybrid solid-state materials with bright future due to their permanent porosity and high thermal stability. The use of these materials ranges from gas storage, separation and catalysis, to a number of diverse potential applications, including optoelectronics, sensors, smart membranes etc. Also aiming at applications in catalysis we have introduced the solvent-free gas-phase loading of MOFs via the adsorption of different volatile organometallic all-hydrocarbon precursors such as ferrocene, cobaltocene and their derivatives. Loading of the MOFs with different metal-organic guests opens a door for development of novel materials with tunable properties. Up to now, only a few examples of detailed structural characterization of the inclusion compounds like Guest@MOF have been described in the literature [1]. We have previously obtained adsorbate structures for numbers of inclusion compounds based on the home powder X-ray diffraction [2, 3]. Here, we present the results obtained in the course of analysis of the guest's ordering and packing inside the 1D-channels of two MOFs, $[\text{Al}(\text{OH})(\text{bdc})]_n$ and $[\text{V}(\text{O})(\text{bdc})]_n$. As revealed, these two topologically similar structures have different adsorption properties. $[\text{Al}(\text{OH})(\text{bdc})]_n$ shows a well-pronounced breathing effect on the contrary to $[\text{V}(\text{O})(\text{bdc})]_n$ which demonstrates neither breathing effect nor appreciable guest capacity. To note, $[\text{Al}(\text{OH})(\text{bdc})]_n$ exhibits a high loading rate