Efficient purification of 1,3-butadiene

Subject Code: B01

With the support by the National Natural Science Foundation of China, the research team led by Prof. Zhang Jiepeng (张杰鹏) at the MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry, Sun Yat-Sen University, recently reported a new adsorptive separation mechanism for efficient purification of 1,3-butadiene in *Science* (2017, 356: 1193—1196).

As the fourth most produced chemical product, 1,3-butadiene is usually separated from C4-hydrocarbon mixtures (primarily consisting of 1,3-butadiene, 1-butene, isobutene, and butane). Because of the close proximity of their boiling points and the heat sensitivity of 1,3-butadiene, the purification is very difficult. In industry, 1,3-butadiene is typically isolated by extractive distillation using, which is not only very energy consuming but also environment-unfriendly as organic solvent and polymerization inhibitor are needed. Differential adsorption by porous materials may be used to separate C4 hydrocarbons at ambient temperature and pressure, but they prefer to adsorb the 1,3-butadiene (smallest size and highest polarity) with low selectivity (small differences), which requires multiple adsorption-desorption cycles to achieve an acceptable 1,3-butadiene purity.

Zhang's group proposed to use quasi-discrete pores to control the conformation of flexible C4-hydrocarbons and reduce the adsorption enthalpy of 1,3-butadiene by its relatively large energy penalty for conformational change. They systematically compared the C4-hydrocarbon separation behaviors of 10 representative porous coordination polymers (metal-organic frameworks), and used single-crystal X-ray diffraction and multilevel computational simulations to prove this concept. Meanwhile, they found MAF-23 as the first porous material exhibiting the reversed adsorption/separation sequences for C4 hydrocarbons, which allows 1,3-butadiene to elute first in the fixed-bed adsorber operated at ambient temperature and pressure, giving high purity of 99.9%+.

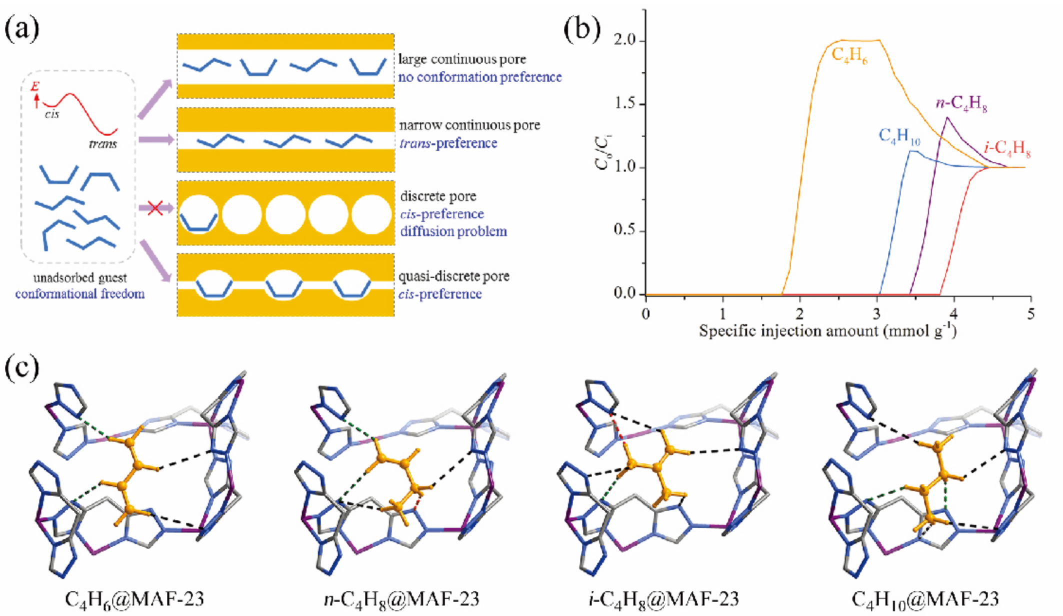

Figure (a) Controlling the guest conformations by variation of the pore size, shape, and dimensionality. (b) Breakthrough curves of MAF-23 for 5 : 2 : 2 : 1 mixture of C_4H_6/n-C_4H_8/i-C_4H_8/C_4H_{10}. (c) Host-guest interactions revealed by single-crystal X-ray diffraction.