World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

Quantum Sieving for Hydrogen Isotope Separation

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Abstract : One of the challenges in modern separation science and technology is the separation of hydrogen isotopes mixtures since D2 and H2 consist of almost identical size, shape and thermodynamic properties. Recently, quantum sieving of isotopes by confinement in narrow space has been proposed as an alternative technique. Despite many theoretical suggestions, however, it has been difficult to discover a feasible microporous material up to now. Among various porous materials, the novel class of microporous framework materials (COFs, ZIFs and MOFs) is considered as a promising material class for isotope sieving due to ultra-high porosity and uniform pore size which can be tailored. Hence, we investigate experimentally the fundamental correlation between D2/H2 molar ratio and pore size at optimized operating conditions by using different ultramicroporous frameworks. The D2/H2 molar ratio is strongly depending on pore size, pressure and temperature. An experimentally determined optimum pore diameter for quantum sieving lies between 3.0 and 3.4 Å which can be an important guideline for designing and developing feasible microporous frameworks for isotope separation. Afterwards, we report a novel strategy for efficient hydrogen isotope separation at technologically relevant operating pressure through the development of quantum sieving exploited by the pore aperture engineering. The strategy involves installation of flexible components in the pores of the framework to tune the pore surface.

Keywords : gas adsorption, hydrogen isotope, metal organic frameworks(MOFs), quantum sieving
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020