Molecular dynamics simulation study on characterization of bis (triethoxysilyl)-ethane and bis(triethoxysilyl)ethylene derived silica-based membranes

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ABSTRACT

The virtual structures of organic–inorganic hybrid silica membranes were prepared on a computer by introducing two different types of organic functional groups into a conventional silica network. bis(triethoxysilyl)ethane (BTESE) and bis(triethoxysilyl)ethylene (BTESEthy) derived silica-based organic–inorganic hybrid microporous materials were modeled and their structures such as pore size distribution and radial distribution function were studied. Adsorbability of water and diffusivity of helium molecule was also examined. Both the hybrid silica structures showed larger pore size than pure silica. The difference in water adsorption performance and helium diffusivity was observed between two types of hybrid silica structures. BTESEthy silica showed higher loading of adsorbed water and it is expected to be a promising material for water treatment. Helium diffusivity in BTESEthy silica was greater than that in BTESE silica, which was in consistent with the micropore size.

Keywords: Molecular dynamics; Hybrid membrane; Water adsorption; Gas diffusivity