東京大学グローバルCOEプログラム　機械システム・イノベーション国際拠点

東京大学 THE UNIVERSITY OF TOKYO

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Adsorption / diffusion of guest molecules in zeolites / MOFs studied by molecular simulations

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要旨

Molecular simulations of adsorption and diffusion in zeolites and Metal Organic Frameworks Zeolites are important materials in the petrochemical industry; they are used as catalysts and in separations. A detailed understanding of adsorption and diffusion at the molecular scale is important for anoptimal use of a zeolite in a particular applications. Molecular simulations are an excellent tool to obtain such an understanding. In my presentation I will present several examples of this, in particular for the adsorption and diffusion of water and alcohols in hydrophobiczeolites. This information is important for the separation of water/alcohol mixtures in zeolite membranes.

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