Adsorption and desorption surface dynamics of gaseous adsorbate on silicate-1 by molecular dynamics simulation

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Résumé

The dynamics of adsorption and desorption of gaseous molecules on the external surface of a crystal and a membrane of zeolite silicate-1 is investigated by molecular dynamics simulation. The gases are argon and three hydrocarbons, n-heptane, n-butane and ethylene. The sticking coefficient and the desorption coefficient are calculated for different coverages and presented.

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