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Time dependent self-diffusion coefficient of molecules in porous media

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Abstract

Using Monte Carlo simulation, the time dependence of the self-diffusion coefficient D(t) in porous media was investigated. It was found to be a decaying function with a cut-off to zero at time t. The exact form of decay depended on the details of the geometry of porous space. The details of the geometry were described by the surface orientation autocorrelation function. The short-term behavior of D(t) was governed by the surface population of the molecules.

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