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Lévy walks of strong adsorbates on surfaces: Computer simulation and spin-lattice relaxation

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Abstract

Using a Monte Carlo method, the time dependence of the mean-squared displacements along planar and spherical liquid-solid interfaces and the displacement distribution were simulated for a random walker. In the strong-adsorption-short-displacement limit, the Cauchy propagator typical for Lévy walks was verified. It is shown that the displacements effectively taking place along surfaces follow a superdiffusive time dependence of the mean square. Surface diffusion is the crucial process of the "reorientations mediated by translational displacements" mechanism of spin-lattice relaxation. This is demonstrated by considering a strongly adsorbed molecule population on spherical surfaces or on planar surface patches representing a certain finite orientation correlation length. The conclusion is that Lévy walks on curved surfaces account for the experimental findings obtained with field-cycling NMR relaxometry, whereas strongly adsorbed molecules escaping to the bulk liquid play a minor role.