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Showcasing research from the group of Prof. Michael Finnis, Imperial College London, UK and Prof. Ralf Metzler, University of Potsdam, Germany.

The diffusion of doxorubicin drug molecules in silica nanoslits is non-Gaussian, intermittent and anticorrelated

This paper reports the results of all-atom Molecular Dynamics simulations of a doxorubicin molecule diffusing in water and confined to a nanoscale silica channel. Our statistical analysis reveals anomalous diffusion, due to strong interactions with the surfaces of the channel, and exhibiting a mixture of characteristic features. These include non-Gaussian and anticorrelated displacements, non-ergodic diffusion, and pronounced ageing. The results would be relevant to modelling a system of drug-delivery via nanoporous silica particles.