

Ion and Molecule Transport in Surface Functionalized Nanopores - a NMR Study

M. Vogel¹ and S. Schneider¹

¹*Technische Universität Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany
E-mail: sschneider@nmr.physik.tu-darmstadt.de*

We analyze ion and molecule transport in peptide-functionalized nanopores. This endeavor aims to assist a development of a new generation of nanosensors, which combine biological and synthetic nanopores. While being highly selective and sensitive, biological ion channels lack the robustness for technological applications. Contrarily silica pores are well proven in industrial and clinical environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favorable properties of both fields.

To optimize such pores, it is of strong interest to understand the influence of various confinements on the ion and molecule transport inside. Such confined dynamics depend on the pore geometry and the guest-host interactions determined by the properties of the inner surfaces. We vary these parameters systematically, in particular by peptide functionalization of silica surfaces, and study their effects on the dynamics by NMR. We combine various NMR techniques which provide access to local dynamics, with NMR approaches in field gradients to measure self-diffusion coefficients. These methods proved well suited to analyze the dynamics of pure water [1,2]. Here, we apply them to aqueous salt solutions in bulk and nanopore confinement. The experimental setups include ¹H and ²H NMR to investigate water dynamics as well as ⁶Li and ²³Na NMR to analyze the diffusion of various ionic species.

We find a strong slowdown of both local dynamics and translational diffusion in confinement. Temperature dependent T₁ relaxation measurements to analyze local dynamics reveal that the T₁ minimum for the confined system appears at higher temperature compared to the bulk solution, indicating the slowdown. In translational diffusion this is seen by smaller diffusion coefficients in MCM-41 easily by an order of magnitude, e.g. 1e-11 m²/s in bulk and 1e-12 m²/s in confinement at 210K. However, the extent of the slowdown and the relation between short- and long-range dynamics substantially depends on the confinement properties.

References

1. M. Sattig and M. Vogel, *J. Phys. Chem. Lett.* **5**, 174 (2013).