# Signatures of Single-File Diffusion in Dipeptide Nanotubes by Xe-129 Pulsed Field Gradient NMR

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## Introduction

A fundamental understanding of transport of gaseous sorbates in systems of one-dimensional nanochannels is important for a number of applications, including catalysis, separations, and nanofluidics. Confinement to one-dimensional channels can lead to anomalous single-file diffusion, i.e. diffusion under conditions when sorbate molecules cannot pass one another in narrow channels. In this case, the mean square displacement (MSD) grows proportionally to the square root of the diffusion time for a broad range of diffusion times. Although the number of publications on computational studies of single-file diffusion has grown very rapidly over the past decade, there are only a few experimental reports of the observation of such transport. In this project we have obtained pulsed field gradient (PFG) NMR data pointing at single-file diffusion of xenon gas confined inside dipeptide nanotubes.

## Experimental

Self-assembled L-Ala-L-Val (AV) and L-Val-L-Ala (VA) dipeptide nanotubes were used as sorbents. Studies of Xe diffusion in these systems were performed by $^{129}$Xe PFG NMR using a wide-bore 17.6 T Bruker BioSpin spectrometer located at AMRIS, University of Florida. Magnetic field gradients with amplitudes up to 30 T/m were generated using a diff60 diffusion probe and Great60 gradient amplifier (Bruker BioSpin).

## Results and Discussion

**Figure 1** shows the time dependences of the MSD of Xe measured by $^{129}$Xe PFG NMR in dipeptide nanotubes at 298 K. It is important to note that even for the largest diffusion time used the root MSDs of Xe atoms inside nanotube channels were at least one order of magnitude smaller than the average length of the nanotubes (around 50 micrometers). The experimental data in the figure obey the time scaling of single-file diffusion (MSD $\propto t^{1/2}$). This observation is consistent with the expectation that Xe atoms are too large to pass one another in the channels of AV and VA nanotubes. The PFG NMR observation of the time scaling of single-file diffusion could be caused by normal diffusion in nanochannels that bend and form coils. This and other possible alternative explanations of the observed time scaling of SFD are ruled out by previously published hyperpolarized tracer exchange data in AV nanotubes [1]. In the tracer exchange experiments, the increase in concentration of hyperpolarized xenon atoms inside the channels is observed as a function of time (τ) under the conditions when the concentration of all (polarized plus unpolarized) Xe atoms in the channels remains the same at all times.

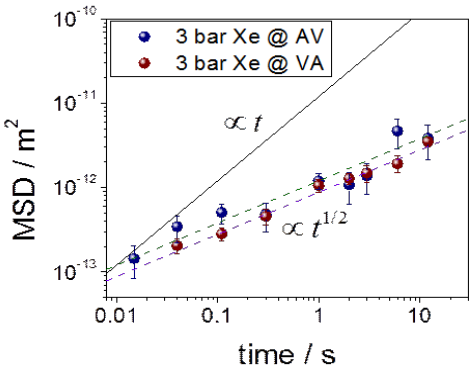


**Figure 1.** Examples of the measured dependencies of the mean square displacements of Xe atoms inside AV and VA nanotubes on diffusion time at 298 K.

## Conclusions

$^{129}$Xe PFG NMR was used to obtain evidence of single-file diffusion of Xe in dipeptide nanotubes.

## Acknowledgements

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## References

[1] Bowers, C.R., *et al*., AIP Conf. Proc. **1330**, 43-46 (2011).