Proton Transport through Peptides Nanotubes

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Peptide nanotubes consist of cyclic peptides piled on top of each other and held together by hydrogen bonds, making them similar to carbon nanotubes in morphology and aspect ratio. These materials are interesting both from the fundamental point of view and for the possible technological applications. They have been employed in biocompatible devices and as drug-delivery agents and are also promising proton conducting materials for the development of fuel cells, batteries, sensors and other advanced technologies. However, proton transport in peptide nanotubes is far from being well understood. Recent experiments on cyclic octa-peptides based on phenylalanine and functionalized with either lysine, arginine or histidine [1] showed an-order-of-magnitude-larger proton conductivity for the lysine-containing nanotubes. Theoretical simulations there included ascribed this to the different flexibilities of the side chains. However, what the role of the surrounding water molecules is on the proton transport through these systems had not been clarified. Inspired by these results, therefore, we carried out molecular dynamics simulations on these systems in aqueous environment to try gaining an insight into how water molecules can mediate the proton flow. For that, we considered various possibilities, considering both isolated nanotubes and bundles, which are known to be formed in the experimental self-assembled structures.

References

[1] S. Roy, L. Zheng, O. Silberbush, M. Engel, Y. Atsmon-Raz, Y. Miller, A. Migliore, D. N. Beratan, and Nurit Ashkenasy, J. Phys. Chem. B (2021), 125, 46, 12741–12752l.

Figures

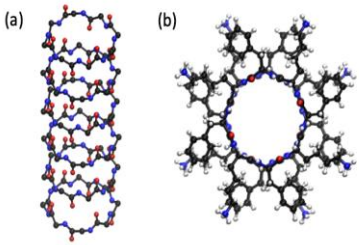

Figure 1: Side (a) and top views (b) of a section of the peptide nanotube c(KF)4; in (a) only the backbone is shown for clarity (*i.e.* the lysine (K) and phenylalanine (F) side chains are not shown). Each peptide ring contains 4 K and 4 F amino acids in an alternate fashion.