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Nanoconfinement: from nanotubes to biological channel

Nanoconfinement is the presence of small molecules within nanoscales cavities. In this talk we will explore the effects of nanoconfinement in synthetic and natural pores via molecular dynamics simulations. For the former we will show how narrow carbon nanotubes are able to load water and small alcohols due to entropic effects. For the latter, we will show how by just exploring the hydration profiles from the voltage sensors of the BK ion channel, one is able to predict the molecular determinants responsible for voltage sensing; finally we will show how relatively small changes in pore diameters of aquaporins due to changes in membrane tension can have macroscopic repercussions.