WEEKLY SEMINAR

Topic: **Gating, Pumping and Signal Conduction Mediated by Water Molecules Confined in Nanoscale Space Studied by Molecular Dynamics Simulations**

Speaker: **Prof. Haiping Fang**
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Time: 15:30-16:30, 11 March, 2014

Venue: Room153, Geography Building, 3663 Zhongshan Road North, Shanghai

(华东师范大学中山北路校区，地理楼 153 室)

ABSTRACT OF THE TALK

Water confined in nanoscale space usually exhibits behavior different from bulk systems due to the ordering of the hydrogen bonds, and the understanding is of great importance in the studies of the biological activities, wetting behavior and the designing of novel molecular devices/ machines/ sensors. Here, we present some of our recent progress using molecular dynamics simulations. Water permeations across the nanochannels show excellent electric and mechanical on-off gatings when the water inside the channels forms single-file structures. We found unidirectional water transportation when there was a combination of charges positioned adjacent to a nanopore, inspired from biological water channels, Aquaporins. Further, due to the concerted charge dipoles of the single-file water, signal can be transmitted, converted and multiplified along the nanochannels. We also show that the biomolecules with aqueous liquids inside a single-walled nanotube can be controllably manipulated by using external charges outside the nanotube, which is expected to serve as lab-in-nanotube. Finally, we show the unexpected phenomenon of “water that does not completely wet water monolayer” at room temperature due to the ordered water monolayer of the first water layer on the solid and bio-related surfaces which had been partly confirmed by experiment very recently.

BIOGRAPHY

Haiping FANG is a Senior Research Scientist and Director of the Division of Interfacial Water at the Shanghai Institute of Applied Physics, Chinese Academy of Sciences. He received his Ph.D. in theoretical physics from the Institute of Theoretical Physics, Chinese Academy of Sciences in 1994. His current research interests include the behavior of statistical physics at the nanoscale, interfacial water and its biological significance, stability and dynamics of nanobubbles and nanobubble-protein interactions, and liquid water anomalies. He has more than 100 journal publications and 3 patents. He won the 100 Talents Program of the Chinese Academy of Sciences in 2002, National Science Fund for Distinguished Young Scholars in 2008, and Shanghai Leading Academic Discipline Project in 2009. Currently he serves as the editorial board member for Scientific Report.