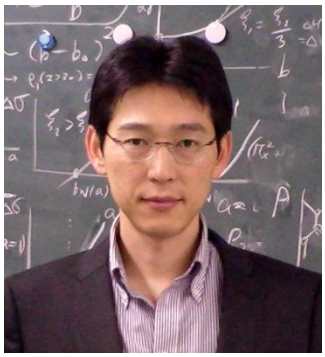
北京大学量子材料科学中心

International Center for Quantum Materials, PKU

ICQM Weekly Seminar

Hydrophobes in Water / Water in Nanotubes



Kenichiro Koga

Department of Chemistry, Okayama University

Time: 4:00pm, Dec19, 2012 (Wednesday)

时间：2012年12月19日 （周三）下午4:00

Venue: Room 607, Conference Room A , Science Building 5

地点：理科五号楼607会议室

Abstract

Three topics on water are presented: (1) A general view on hydrophobic hydration; (2) Do methane molecules attract each other in water?; and (3) Phase transitions of water in carbon nanotubes. The first two are ongoing projects including unpublished works while the third is a brief review of what we have done on confined water.

(1) The solvation characteristic of the hydrophobic hydration is realized even in simple liquid mixtures. In the constant-volume solvation process the solvation thermodynamics of nonpolar solutes in water and that of nonpolar solutes in a simple liquids are found to be qualitatively similar to each other. The significant difference between the two systems arises in the constant-pressure solvation. The origin of the difference is directly related to the smallness of the thermal pressure coefficient of water at low temperatures.

(2) The osmotic second virial coefficient of methane in water is calculated by evaluating the Kirkwood- Buff integral of the solute-solute pair correlation function h(r). In a range of temperature from 258 K to 373 K, the osmotic virial coefficient is a deceasing function of temperature, with its values nearly zero in supercooled water and close to −0.13nm3 at 373 K. The trend is consistent with a view that the hydrophobic attraction is weak or absent at low temperatures and becomes significant only at high temperatures.

(3) Of the properties of water in the well-defined nanopores, a fundamental yet little known was a global picture of the phase behavior. Previous results of other substances imply that neither the melting point nor the freezing behavior of a substance changes monotonically with the pore diameter and they are extremely sensitive to the diameter. Here we report the result of MD simulations of water in wide ranges of the nanotube diameter and temperature, and then propose a global phase diagram for water in carbon nanotubes with diameter ranging from 9 to 17 Å.

About the Speaker

Professor Kenichiro Koga was born November 20, 1968 and raised in Kyoto, Japan. He received his bachelor's degree at Osaka University (1991), his master's degree at Kyoto University (1993) and Ph.D at Kyoto University (1996). He then joined Professor X. C. Zeng's group as a postdoctoral fellow at University of Nebraska-Lincoln (1996-1999). He was appointed Lecturer (1999) and Associate Professor (2000) at Fukuoka University of Education. He was awarded the JSPS Fellowship for Research Abroad and visited Professor B. Widom at Cornell University (2001-2003). He was appointed Associate Professor (2003) and Professor (2009) at Okayama University. He is interested in problems in statistical mechanics of liquids and fluid interfaces. This includes such subjects as phase equilibria and phase transitions in bulk and confined systems, the hydrophobic effect, nucleation and surface tension. Main theoretical tools are statistical mechanics, thermodynamics, and computer simulation.