ACCMS-Global Research Center
SRMIST, Chennai India

Webinar #18

Prof. Vladimir R. Belosludov

Institute of inorganic chemistry, Siberian Branch, RAS

Title: Unexpected formation of methane clathrate hydrate in supersaturated methane solution at low pressure

Registration link: https://tinyurl.com/3d8pe769

**Zoom details will be shared with the registered participants*

27 June 2023, 12.30 – 2.00 pm Indian Standard Time

Short biography

Prof. Vladimir Belosludov is Head of laboratory of thermophysical foundations of gas hydrate technologies in Novosibirsk State University. He is also a professor of physics in Institute of inorganic chemistry, Siberian Branch, RAS. VR Belosludov is a well-known specialist in the field of solid state theory and physical chemistry. His research is devoted to solving problems related to the structure and properties of various types of substances such as superionic conductors, ferroelectrics, water, clathrate compounds and complex molecular crystals of metal β-diketonates. He has published about 260 papers in peer-reviewed reputed journals with more than 5400 citations. The highlights of his pioneer works are follows. A molecular model of clathrate compounds was constructed, formed by guest molecules included in the cavities of the host lattice. This model made it possible to understand the fundamental importance of the interaction of guest molecules with each other and with the host lattice for describing the thermodynamic properties of clathrate compounds. The properties of water at the molecular level, the existence of nano-sized structural inhomogeneities embedded in the dynamic network of H-bonds was discovered for the first time.

Abstract

Gas hydrate formation mechanism at early stages is still under discussion. At present time there are two main mechanisms describing this process on molecular level. The first one is the labile cluster hypothesis and the second one is the local structure hypothesis. The main difference between these concepts is the priority of local or volume hydrogen bond (H-bond) network arrangement.

By this work we give insight of water structure ordering preceding the formation of first hydrate-like structures and its time evolution. Using molecular dynamics the evolution of a metastable solution for "methane + water" was studied for 3.36, 6.5, 9.45, 12.2 and 14.8 mol% methane concentrations at 270 K and 1 bar during 100 ns. We have shown that the process of hydrate formation is a collective process. At the initial stage (0-1 ns) H-bond network of metastable solution of various methane concentrations reorganizes and the first fluctuating cavities appear. Thus, the coexistence of the hydrate phase with water solution is shown in a system with methane concentration in water ~7–9 mol% metastable water solution. At higher methane concentrations (12 mol% and more) phase separation is observed with the formation of nano-bubbles of methane gas. At lower methane concentration (5 mol% and less) there are no signs of gas phase separation or hydrate-like structure formation over the 200 ns. We associated the start of hydrate formation with preceding increase of tetrahedrality of each water molecule local order calculated by the means of F_3/F_4 order parameters. The molecules with the high degree of tetrahedrality are distributed in volume uniformly. The formation of small and large fluctuation of sI cavities is shown before the steady hydrate growth begins. Later, the constantly presented hydrate cavities become the basis for few independent hydrate nucleation centers. This new mechanism of hydrogen bond network reorganization depends on the entropy of the cavity arrangement of the guest molecules in the hydrate lattice and leads to the hydrate growth.

Panelist

Prof. Kaoru Ohno

Yokohama National University

Japan

Convener:

Prof. Yoshiyuki Kawazoe
Head, ACCMS-GRC
SRMIST, KTR

Organizers:

Dr. V.J.Surya & Dr.S. Yuvaraj
ACCMS-GRC Center-in-Charges
Dept. of Physics and Nanotechnology, SRMIST, KTR

NAAC A++ | Category 1 with 12B Status | (2022) Ranked 19th University | (2023) World Ranking one among 41 Indian Universities | (2023) World Ranking one among 75 Indian Universities | (2021) Ranked 4th | (2023) World Ranking one among 14 Indian Universities