\*Department of Chemical Engineering, IIT Kanpur\*

\*SEMINAR\*

Speaker: Dr. Suresh K. Bhatia, Professor, School of Chemical

Engineering, University of Queensland, Australia

\*Topic: How Water Adsorbs in Hydrophobic Nano-spaces \*

\*Date\*\*:\* \*Wednesday \*\*14^th March 2012\*

\*Place: L-1\*

\*Time:16:00 to 17:00\*

\*All are welcome\*

Tea will be served at 15:45 near the venue

\*\*\*Abstract:\*

The understanding of the mechanism of water adsorption in the

hydrophobic nanospaces of carbons is critical to many industrial

processes for gas separation and water purification, and to emerging

nanotechnologies for desalination, CO2 capture from flue gas, and

separation by nanofluidic devices. While there have been numerous

attempts at simulating water adsorption in hydrophobic carbons using

idealized models of independent slit pores, only qualitative agreement

with experiment has been achieved, and the answer to the difficult

question of how water enters such spaces has remained elusive. Using

grand canonical Monte Carlo (GCMC) simulations with a realistic model of

a disordered hydrophobic carbon, we show that the key to the puzzle is

the connectivity of the structure -- overlooked by independent slit pore

models. Our simulations and data confirm that significant amount of

water adsorbs below the saturation pressure in purely hydrophobic

nanopores, and it is demonstrated that this occurs only when pore

entries are sufficiently large to allow the passage of stable

hydrogen-bonded water clusters. We investigate the effect of pore

connectivity through synthetic models of connected and unconnected slit

pores, and show that the connectivity to narrow water-filled pores

mediates the adsorption of water in large hydrophobic nanospaces. This

unique feature is not observed for nonpolar or weakly polar gases (e.g.

Ar or N2) at subcritical conditions, and explains why the Kelvin

equation fails to estimate the condensation pressure for water. The

results open the door for the design and tailoring of efficient

adsorbents for CO2 capture, in which the co-adsorption of water vapor

which saturates flue gas is inhibited.\*

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\*About the Speaker\*

\*\* Suresh Bhatia received his undergraduate degree in chemical

Engineering from the Indian Institute of Technology, Kanpur, and

Master's as well as PhD degrees from the University of Pennsylvania. He

worked with the consulting firm of Booz Allen and Hamilton, as well as

with Mobil R&D Corpn., in the USA, before joining academia. He began his

academic career at the University of Florida, where he worked for two

years, and in 1984 he joined the Indian Institute of Technology, Mumbai,

and subsequently the University of Queensland in 1996. His main research

interests are in adsorption and transport in Nano-porous materials and

in heterogeneous reaction engineering, where he has authored over one

hundred and ninety scientific papers in leading international journals.

He is recognised for his advances in the modeling of gas-solid

reactions, in the transport of fluids in Nano-porous materials, in the

Nano-scale characterization of carbons, and in adsorptive storage.

He has been an invited keynote or plenary speaker at numerous

international conferences, and is the Regional Editor of the

international journal Molecular Simulation.He is a Fellow of two major

academies- The Indian Academy of Sciences, and the Australian Academy of

Technological Sciences and Engineering -- and of the Institution of

Chemical Engineers. He has received numerous awards for his research

including the Herdillia Award, and the Shanti Swarup Bhatnagar Prize for

Engineering Sciences.In 2007 his research on Nano-porous materials was

recognized by Micromeritics Corpn. through its Instrument Grant Award.

He is the only non-American to have received this award, and in 2009 he

received the ExxonMobil Award for Excellence in Chemical Engineering

from the Institution of Chemical Engineers. Since 2010 he holds an

Australian Professorial Fellowship from the Australian Research Council,

and in 2011 he received the inaugural Vice-Chancellor's Award for

Research Excellence at the University of Queensland.

He has served as Head of the Chemical Engineering Division at UQ

between 2007 and 2009, and was instrumental in its elevation to a School

of Chemical Engineering, including within its fold Metallurgy,

Biological Engineering and Environmental Engineering.