Combined Molecular Dynamics and Experimental (AFM, XPS, Neutron Scattering) Analysis of the Biomolecules (DNA, Peptides) Interactions with TiO_2 and related Surfaces

(18^{th} July – 22^{nd} July)

Overview

Understanding the physical and molecular mechanism of the interaction of surfaces, nano and microparticles with DNA represents a great interest in today`s biomedical applications (as implants and sensors), in medicine (diagnostic and treatment of oncology diseases), so on. In this regard, the DNA - NP (nanoparticles) and DNA - metallic surfaces, like as titanium dioxide, TiO_2 are important research targets. Molecular Dynamics simulation has emerged as a powerful tool for studying the interaction and visualizing the problem more closely. A lot of experimental techniques namely, AFM, XPS, Neutron Reflectometry are being extenssivly used in these field to map the predicted results form MD simulations. This is a continuously evolving subject of research with truely interdisciplinary nature, which need more attention from all fields of expertise.

This advance course will cover throughly all the perspectives discussed above and develop scientific understanding to solve the problems related to the field.

Modules	Built up multiply molecular dynamics models for the DNA and titanium dioxide nanosystem Providing MD simulation analysis data to existing molecular models Performing the computational methodology and theoretically analysis approach. Experimental realizations of neutron beam irradiation of the DNA–TiO_2 samples Performing AFM and XPS analysis for the irradiated samples of the interest
Target Audience	Students of all levels (B.Tech/M.Tech/M.Sc/Ph.D) / Faculty members / Researchers from universities and technical institutions.
Fees	Participants from Abroad ------ $300 Students (pursuing Ph. D) ------ Rs 1000 Students (pursuing Masters / Bachelors courses) ------ Rs 1000 Faculty members / Researchers ------ Rs 3000 The above fee includes a working lunch, all instructional materials and computer use for tutorials. The participants will be provided with suitable accommodation on payment basis.

International Resource Person

Prof. Kholmirzo T. Kholmurodov is a Leading Scientist of the Frank Laboratory of Neutron Physics, JINR & Professor of Dubna State University, Dubna-Moscow region, Russian Federation.

He was a visiting professor at Keio University (Yokohama-Kanagawa; 2005-2015), Waseda University (Shinjuku-Tokyo; 2012-2013), Kyoto University (2013-2014), Nagoya University (1997-1998), worked at RIKEN (The Institute of Physical and Chemical Research, Japan, 1998-2003); and was a member of the Japanese Physical Society (2000-2003) and Computation Collaborative Project 5 (the United Kingdom).

He has in his credit more 90 scientific papers, and many reviews.

He is also a member of the ACS (American Chemical Society (ACS); ACS Division of Biological Chemistry,), and an Editorial Board Member of The Open Nanomedicine Journal (Editorial Advisory Board Member).

He is the Editor of several Abstracts and Proceedings Books, from Nova Science Publishers (N.Y.)

Venue: Dept of Physics NIT Patna

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