Computational Studies of Formation and Propagation of Amyloids

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Time: 11:00 am (tea reception: 10:45 am)
Venue: 1614
Academic 2
City University of Hong Kong

General Enquiry: 3442 7413

Chair: Dr J Fan (34429978 junfan@cityu.edu.hk)

~ ALL ARE WELCOME ~
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ABSTRACT

Presence of amyloid fibrils is a hallmark of Alzheimer’s and many other metabolic or neurodegenerative diseases. However, in the case of Alzheimer’s disease, not the insoluble fibrils appear to be the primary neurotoxic agent, but rather small soluble oligomers formed either on-pathway to fibril assembly or off-pathway. Hence, for the purpose of deriving and evaluating treatment options it is important to understand how the equilibrium between the polymorphous fibrils and oligomers is shifted by mutations, changing environmental conditions, or in the presence of prion-like amyloid strains. Probing these processes in experiments or on a computer presents a challenge. Simulations suffer from the problem that the assembly of misfolded proteins into oligomers and fibrils happens on time scales which often cannot be covered in all-atom simulations. We have proposed to overcome this problem by a Replica-Exchange with Tunneling method. We will discuss this approach and present recent work discussing amyloid formation and propagation.

Selected Publications:

BIOGRAPHY

Professor Hansmann received his MA in Philosophy, “Diplom” (equivalent to a MS) and PhD in Physics from the Freie Universität Berlin at Berlin, Germany. He is Professor at the Department of Chemistry and Biochemistry at University of Oklahoma, Norman, OK. From 2005-2007 he held an additional appointment as head of the “Computational Biology and Biophysics” group in the John von Neumann Institute for Computing (Germany’s premier supercomputer center). In 2008 he was inducted as a Fellow of the American Physical Society. Dr. Hansmann leads an active research program in areas of development of global optimization techniques and modeling of biomolecular and complex systems. His work is supported by both National Science Foundation and the National Institutes of Health (USA). Dr. Hansmann has authored and co-authored more than 200 publications which receive 200-300 annual citations. His H-index is 32. He organizes since 2006 a series of annual workshops titled “From Computational Biophysics to Systems Biology”.