SEMINAR

Department of Biological Sciences

NUS National University of Singapore

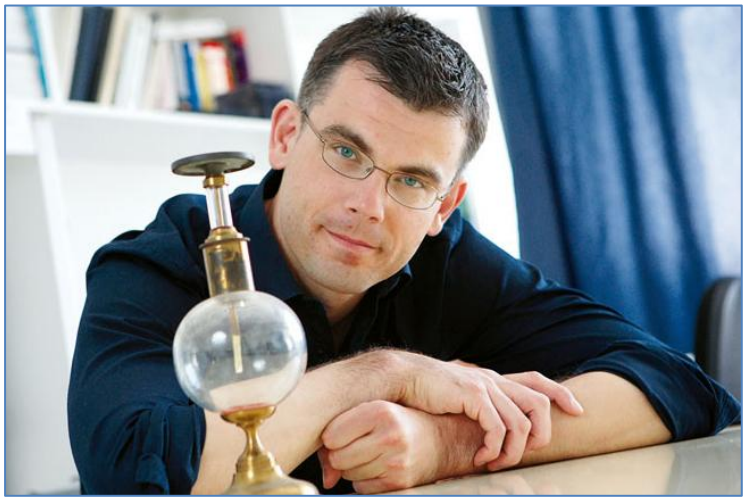
Tues, 31 Jul 2012 | 4pm | Seminar Room S1A-02-17

Hosted by A/P Henry Mok

Studying protein-protein interactions using computer simulations: from specific effects to protein ecology

Computational modeling of biomolecular structure and dynamics has become an indispensable aid in our efforts to understand biological events at the molecular level. In this talk, I will focus on using computational approaches to study protein-protein interactions. Direct non-covalent protein-protein interactions underlie most of biological functional activity on the molecular level. Despite significant progress in studying these processes, a number of open questions remain. How do the partners find each other in the crowded and interaction-rich cellular environment?

What is the role of co-localization in binding and what are the mechanisms that lead to it? What are the exact mechanisms of the specific recognition of binding surfaces? I will present several recent results obtained using structural modeling and molecular dynamics simulations to address these questions. In particular, I will focus on: 1) the question of binding specificity in ubiquitin binding, 2) the influence of general physicochemical properties of proteins on their localization and interactions, and 3) the role of conformational entropy in protein binding.



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