School of Molecular Sciences
Arizona State University

SMS Spring 2022 Seminar Series

Friday Feb 4 | 2:30pm | Virtual

Maximum Likelihood Analysis in Single-Molecule FRET

My presentation consists of two parts. In the first part, I give a brief overview of the theoretical methods we use to analyze single-molecule FRET experiments. Single-molecule Förster resonance energy transfer (FRET) between fluorescent donor and acceptor labels attached to a protein or nucleic acid is a powerful tool to probe intramolecular distances and to study structure and dynamics of macromolecules. The quantitative analysis of such experiments is particularly challenging when the inter-dye distance fluctuations are fast. We consider each and every photon and use a maximum likelihood method to get the information about fast conformational dynamics. I will show the application of the method to two- and three-color FRET.

In the second part of my talk, I discuss our recent works on the theory of diffusion-influenced reactions. When a reaction is very fast, the reaction rate is influenced by the rate of reactant transport, i.e., the rate at which the reactants find each other. Conventional way to take translational diffusion into account is to modify the rate constants that enter the rate equations of ordinary chemical kinetics. However, in coupled bimolecular reactions such as repeated modification of a multisite protein, not only the rate constants but also the structure of the rate equations (and the corresponding kinetic scheme) can be altered. We developed a theory that allows one to determine the influence of diffusion on the kinetics of a complex network of coupled reactions. I illustrate the use of the theory by two examples, double phosphorylation of a substrate by the same enzyme and cluster channeling in enzymatic cascade reactions.

Irina V. Gopich, PhD

Physicist, Laboratory of Chemical Physics

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Irina V. Gopich is a physicist in the Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, Maryland. Her research interests are in theoretical chemical physics and biophysics. She obtained her undergraduate degree in physics from the Novosibirsk State University, Russia, and PhD in chemical physics from the Institute of Chemical Kinetics and Combustion, Novosibirsk, Russian Academy of Sciences. After a short postdoc with Professor Noam Agmon at the Hebrew University of Jerusalem, Israel, she worked with Dr. Attila Szabo at the National Institutes of Health. Her current research is focused on single-molecule fluorescence spectroscopy and the role of diffusion in multisite binding and enzyme catalysis.

**ZOOM option available: https://asu.zoom.us/j/87081218152*