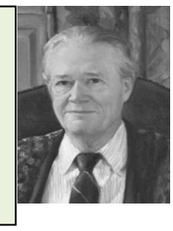
Emerson Center Lectureship Award Symposium

Molecular Level Understanding of Complex Systems

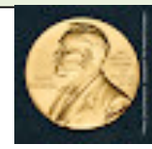


September 23, 2016, Harland Cinema, Dobbs University Center, Emory University

AWARD WINNER &: KEYNOTE SPEAKER

Prof. Arieh Warshel,

University of Southern California



Nobel-2013 Chemistry

How to Model the Action of Complex Biological Systems on a Molecular Level

Despite the enormous advances in structural studies of biological systems we are frequently left without a clear structure function correlation and cannot fully describe how different systems actually work. This introduces a major challenge for computer modeling approaches that are aimed at a realistic simulation of biological functions. The unresolved questions range from the elucidation of the basis for enzyme action to the understanding of the directional motion of complex molecular motors. Here we review the progress in simulating biological functions, starting with the early stages of the field and the development of QM/MM approaches for simulations of enzymatic reactions. We provide overwhelming support to the idea that enzyme catalysis is due to electrostatic preorganization and then move to the renormalization approaches aimed at modeling long time processes, demonstrating that dynamical effects cannot change the rate of the chemical steps in enzymes. Next we describe the use our electrostatic augmented coarse grained (CG) model and the renormalization method to simulate the action of different challenging complex systems, such as F1 ATPase, F0 ATPase, myosinV, and more.

INVITED SPEAKERS

David G. Lynn
Department of Chemistry, Emory University

R. Brian Dyer
Department of Chemistry Emory University

R. Prabhakar
Department of Chemistry, University of Miami

EVENTS SCHEDULE

11:00–12:30	**POSTER PRESENTATIONS**
1:30 – 2:00	**OPENING CEREMONY & AWARD PRESENTATION**
2:00 – 3:00	**Arieh Warshel:** *How to Model the Action of Complex Biological Systems on a Molecular Level*
3:00 – 4:00	**David G. Lynn**: *Emergence of Functional Peptide-Based Polymers in Multi-phase Dynamic Chemical Networks*
4:00 – 4:15	**COFFEE BREAK**
4:15 – 5:15	**R. Brian Dyer:** *The Search for Reactive Conformations in Enzymatic Catalysis*
5:15 – 6:15	**R. Prabhakar:** *Computational Modeling of Reaction Mechanisms, Drugs and Biomaterials*
6:15 – 6:30	**CLOSING**
6:30 – 9:00	**DINNER (by invitation)**

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REGISTRATION: http://www.emerson.emory.edu/conferences/form/register.html

CONTACT: dmusaev@emory.edu: Ph: 404-727-2382

Registration is free. Please register to attend