UCLA College | Physical Sciences Chemistry & Biochemistry

PHYSICAL CHEMISTRY SEMINAR

Prof. Davit Potoyan

Department of Chemistry
Iowa State University

Monday, November 7th, 2022
4:00 PM | YH 4222

Bhaumik Collaboratory
Yoo Seminar & Conference Room

Multi-Scale Computational Studies of Biomolecular Dynamics and Phase Separation

Abstract: Cellular life is contingent on the ability of biomolecules to self-organize by forming dynamic and functional compartments. Uncovering the underlying driving forces for biomolecular self-organization is a long-standing fundamental problem for biological sciences. Experiments of the last decade have found that liquid-liquid phase separation of biomolecules underlies the formation of many mesoscopic cellular compartments. The ability to phase separation is encoded in the sequence of biomolecules. However, in vivo biomolecules are phase-separated in heterogeneous and out of equilibrium environments, further complicating the extraction of simple sequence-function relationships. Disentangling the roles of sequence and environment on biomolecular phase separation poses unique challenges for both theory and experiment, which call for developing novel interdisciplinary multi-scale computational approaches. Our group is developing and applying multi-scale computational models that use atomistic, coarse-grained, and phase-field techniques to study nuclear compartmentalization at different scales, in and out of equilibrium. In the talk, we will present recent results on protein-RNA phase transitions, mesoscale nuclear dynamics of chromatin phase separation, and detailed models of biomolecular condensates based on bioinformatics and atomistic simulations.

Please contact isaiahgtz@chem.ucla.edu for additional information.