Seminar/Talk

Statistical Descriptions of Molecular Phenomena: Circuits, Spectra, and Dynamics

Ravi Venkatramani
Tata Institute of Fundamental Research, Department of Chemical Sciences

Host: Latha Venkataraman

Our research group develops robust, systematic and statistical descriptions of diverse physicochemical phenomena in molecular and biomolecular systems. I will present three new conceptual ideas that have emerged through our efforts in last decade. In the first part of this seminar, I will introduce electronic molecular breadboards as a framework for prototyping circuits within experimental break-junction setups. Here, conductance histograms serve as statistical fingerprints of circuit pathways. Our new computational models that simulate these histograms, enable experimental access to embedded circuits and highlight how statistical descriptions can guide the design of complex functional molecular circuits.Next, I will turn to the discovery of protein charge transfer spectra (ProCharTS), which explains puzzling but consistent detection of non-aromatic UV-vis absorption/emission. Overturning textbook paradigms, we have shown that ProCharTS arises from to charge-transfer transitions within clusters of charged amino acids. Using Time-Dependent Density Functional Theory (TDDFT) on statistical ensembles of charged amino acid clusters, I will show how such novel spectra can be simulated and predicted. ProCharTS opens up a new label-free optical mode to track biologically relevant processes such as post-translational modifications and biomolecular interactions.Finally, I will address the problem of quantitatively sampling rugged biomolecular energy landscapes in in Molecular Dynamics (MD) simulations. Specifically, the introduction of the cumulative variance of coordinate fluctuations (CVCF) as a parameter-free metric to identify Boltzmann-sampled regions of trajectories, and the mode evolution metric (MEM) to detect locally converged directions toward hidden metastable states. These new statistical ideas are integrated into AutoSIM, a software which discovers reaction coordinates and then extracts energy landscapes governing biomolecular transitions.

Wednesday, January 21, 2026 01:30pm - 02:30pm
Sunstone Bldg / Ground floor / Big Seminar Room A / 27 seats (I23.EG.102)

This invitation is valid as a ticket for the ISTA Shuttle from and to Heiligenstadt Station. Please find a schedule of the ISTA Shuttle on our webpage: https://ista.ac.at/en/campus/how-to-get-here/ The ISTA Shuttle bus is marked ISTA Shuttle (#142) and has the Institute Logo printed on the side.