



Seminar/Talk

Protein Motion Beyond Snapshots: Learning from Many Structures to Decode Dynamics

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Host: Alexander Bronstein

Proteins are dynamic machines whose function arises from coordinated atomic motions, yet breakthroughs like AlphaFold remain limited in capturing biomolecular interactions and conformational flexibility due to scarce dynamic structural data. Meanwhile, time-resolved experiments, cryo-electron microscopy and tomography, and high-throughput crystallography generate large datasets of protein motion that remain underused without scalable analysis of structural heterogeneity – limiting efforts to understand mutation effects or design allosteric drugs. Unlocking these questions requires treating experimental datasets not as sources of single structures, but as samples from conformational distributions shaped by time, ligand binding, mutation, and cellular context. To do this, I will detail how we can leverage pre-learned structural understanding from deep learning models to decode conformational dynamics directly from experiment. This vision builds on lessons from ROCKET, an experimental augmentation of AlphaFold that captures biologically meaningful structural variation inaccessible to prediction alone or conventional automated modeling approaches, particularly in low signal-to-noise regimes. I will then explore the hypothesis that, when purposefully engineered, such methods provide a general and scalable framework for integrating experimental observables with biomolecular machine learning, yielding low-dimensional, interpretable representations that reveal mechanistic drivers of protein dynamics.

Thursday, October 22, 2026 02:00pm - 04:00pm

Central Bldg / Ballroom



This invitation is valid as a ticket for the ISTA Shuttle from and to Heiligenstadt Station.

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<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.

