



THE CHINESE UNIVERSITY OF HONG KONG
Department of Physics
SEMINAR

Ensemble Refinement with Cryo-EM Data

by

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Zoom link: <https://cuhk.zoom.us/j/91066372893>



ALL INTERESTED ARE WELCOME

Abstract

Single-particle cryo-electron microscopy (cryo-EM) has recently become a premier method in structural biology for obtaining high-resolution structures of biomolecules. While cryo-EM technically provides single-molecule data for molecules that adopt heterogeneous conformations, most existing reconstruction tools cannot retrieve the ensemble distribution of possible molecular configurations from these data. In this talk, I will introduce our recently developed Bayesian ensemble refinement framework to overcome the limitations and estimate the ensemble density from a set of cryo-EM particles by reweighting a prior conformational ensemble, *e.g.*, from molecular dynamics simulations or structure prediction tools. This framework recovers the equilibrium probability density of the biomolecule directly in conformational space from single-molecule data. It can accurately extract state populations and free energies from a simple toy model and synthetic cryo-EM images of a simulated protein that explores multiple folded and unfolded conformations.