



**The Hong Kong University of Science and Technology**

**Department of Mathematics**

**PhD THESIS EXAMINATION**

**Uncovering the Dynamics of Molecular Systems:  
Structure, Simulation, and Signal**

*By*

**Miss Wenqi ZENG**

**ABSTRACT**

The primary challenge in understanding biological systems lies in deciphering the complex, multi-scale relationships between structure and function. From molecular assemblies to whole tissues, biological structures give rise to dynamic behaviors that are nonlinear, high-dimensional, and often emergent. This thesis presents a unified framework for exploring biological dynamics through four interconnected research directions. Initially, we address protein-ligand binding by predicting ligand poses under spatial and physical constraints, generating biologically realistic conformations that capture molecular interaction dynamics. Building on this, we reconstruct long-timescale biomolecular conformational changes from short simulations, bridging the gap between limited sampling and functional timescales. Next, we analyze single-molecule fluorescence (smFRET) data to reveal hidden dynamic states and transitions from noisy time-series, providing insights into transient molecular behaviors. Finally, we develop a structural sparsity framework using inverse scale space to extract key features from high-dimensional biological data, enabling interpretable models. Together, these directions form a cohesive approach to modeling, learning, and interpreting biomolecular dynamics across spatial, temporal, and statistical dimensions.

**Date : 15 May 2025, Thursday**

**Time : 3:00 pm**

**Venue : Room 4472 (Lifts 25/26)**

**Thesis Examination Committee:**

- Chairman** : Prof. Jidong ZHAO, CIVL/HKUST
- Thesis Supervisor** : Prof. Yuan YAO, MATH/HKUST
- Member** : Prof. Jianfeng CAI, MATH/HKUST
- Member** : Prof. Can YANG, MATH/HKUST
- Member** : Prof. Wenjia WANG, Data Science & Analytics Thrust Area
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*(Open to all faculty and students)*

The student's thesis is now being displayed on the reception counter in the General Administration Office (Room 3461).