IMS-NTU joint workshop on

Biomolecular Topology: Modelling and Data Analysis

(24 Jun 2024–28 Jun 2024)

List of Speakers and Talk Titles

Name & Affiliation	Talk Title
Henry Adams *University of Florida, USA*	Hausdorff vs Gromov-Hausdorff distances
Kathryn Hess Bellwald *EPFL, Switzerland*	Topological perspectives on networks
Ginestra Bianconi *Queen Mary University of London, UK*	The discrete Dirac operator determines the interplay between network topology, geometry and dynamics
Jason Cantarella *University of Georgia, USA*	Linkage and polygon spaces; a test case for TDA?
Gunnar Carlsson *Stanford University, USA*	The TDA User Experience
Chao Chen *Stony Brook University, USA*	Topological Representation and Uncertainty for Biomedical Images
Duan Chen *University of North Carolina at Charlotte, USA*	Geometric structure guided nonnegative matrix factorization model for complete deconvolution of biological data
Jiahui Chen *University of Arkansas, USA*	Geometric data analysis of protein-protein interactions
Yuzhou Chen *Temple University, USA*	Topological Compound Fingerprinting in Computer-Aided Drug Discovery
Herbert Edelsbrunner *Institute of Science and Technology (IST), Austria*	Chromatic persistent homology
Patrizio Frosini *Università di Bologna, Italy*	On the use of group equivariant non-expansive operators for protein pocket detection
Yulia R. Gel *National Science Foundation and University of Texas at Dallas, USA*	Topological Graph Contrastive Learning
Weihua Geng *Southern Methodist University, USA*	A Biophysics DNN Model with Topological and Electrostatic Features

Name & Affiliation	Talk Title
Robert Ghrist *University of Pennsylvania, USA*	Harmonic Methods for Topological Data
Yasuaki Hiraoka *Kyoto University, Japan*	scEGOT: Single-cell trajectory inference framework based on entropic Gaussian mixture optimal transport
Chuan-Shen Hu *Nanyang Technological University, Singapore*	Periodic Geometry and Topology-Based Machine Learning Frameworks in Material Design
Vitaliy Kurlin *University of Liverpool, UK*	Can we geometrically sense the shape of a molecule?
Cristian Micheletti *International School for Advanced Studies (SISSA), Italy*	Designed self-assembly of molecular knots, links and topological gels
Julie C Mitchell *Oak Ridge National Laboratory, USA*	Generative and Coevolutionary Approaches to Protein Structure
Binh Nguyen *Victoria University of Wellington, New Zealand*	Computer vision-inspired graph neural network architectures for molecular property prediction
Jian Tang *HEC Montréal, Canada*	Diffusion Models for Molecular Structure Prediction
Bei Wang *University of Utah, USA*	Capturing Robust Topology in Data
Yuguang Wang *Shanghai Jiao Tong University, China*	The AI Frontier in Protein Design: From Geometric Deep Learning to Large Models
Rongling Wu *Beijing Institute of Mathematical Sciences and Applications, China*	The statistical topology theory of aging
John Z.H. Zhang *Shenzhen University of Synthetic Biology, China*	Toward quantum accuracy in protein energy calculations

This list is accurate as of 27/Jun/2024 and is subjected to changes.