

Applied Topology in Frontier Sciences (11–22 July 2022)

Conference on Topology-based Learning, Biomolecular Topology and
Related Topics



*[Registration](#) is required for this program.

Venue

Virtual: The details and link will be sent to you before the program commences after registration has been processed.



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Conference on Topology-based Learning, Biomolecular Topology and Related Topics (11–15 July 2022)

All times are indicated in **GMT+8**.

For time zones conversion: [Click Here](#)

Monday, 11 July 2022		
Time	Title	Speaker
1950–2000	Opening Remarks	
2000	Session Chair: Julien Tierny (CNRS - Sorbonne Université, France)	
2000–2050	Wasserstein Distances, Geodesics and Barycenters of Merge Trees	Julien Tierny CNRS - Sorbonne Université, France
2050–2140	The dynamics of higher-order networks: the effect of topology and triadic interactions	Ginestra Bianconi Queen Mary University of London, UK
2140–2200	<i>Break</i>	
2200–2250	Spatial representability of neuronal activity	Yuri Dabaghian The University of Texas Health Science Center at Houston (UTHealth), USA
2250–2340	Non-Diffusive Topological Structure of Reactions Dynamics of Complex Molecules and Stochastic Landscapes of Molecular Networks	Jie Liang University of Illinois at Chicago, USA

Tuesday, 12 July 2022		
Time	Title	Speaker
2000	Session Chair: Keith Promislow (Michigan State University)	
2000–2050	Machine learning models for biophysics	Julie Mitchell Oak Ridge National Laboratory, USA
2050–2140	Molecular Sparse Representation by a 3D Ellipsoid Radial Basis Function Neural Network via L1 Regularization	Benzhuo Lu (Absent with apologies) LSEC, Institute of Computational Mathematics, CAS, China Sheng Gui (Represented) LSEC, Institute of Computational Mathematics, CAS, China
2140–2200	<i>Break</i>	

Tuesday, 12 July 2022		
Time	Title	Speaker
2200–2050	Singular-Enthalpic limit for charged diblock polymer blends	Keith Promislow Michigan State University, USA

Wednesday, 13 July 2022		
Time	Title	Speaker
0800	Session Chair: Igor Berezovsky (A*STAR)	
0800–0850	Persistent Spectral Graph and Differential Geometry-Assisted AI for Drug Design	Duc Nguyen University of Kentucky, USA
0850–0940	DNA knotting in liquid crystalline phases	Javier Arsuaga University of California Davis, USA
0940–1000	<i>Break</i>	
1000–1050	Protein allostery: from molecular bases to practical implications	Igor Berezovsky A*STAR, Singapore
1050–1140	Data-driven methods for de novo protein design	Haiyan Liu University of Science & Technology of China, China
1140–2000	<i>Session will resume at 8 pm.</i>	
2000	Session Chair: Xinqi Gong (Renmin University of China)	
2000–2050	Computational study of protein-ligand and protein-protein interactions	Zenghui Zhang, John NYU Shanghai, China
2050–2140	Multibody protein interaction complex structure prediction	Xinqi Gong Renmin University of China, China
2140–2200	<i>Break</i>	
2200–2250	Integrating Machine Learning and Molecular Modeling for Drug Design	Yingkai Zhang New York University, USA
2250–2340	Thermodynamic and Dynamic Properties of Phase-Separated Biomolecular Condensates	Huan-Xiang Zhou University of Illinois Chicago, USA

Thursday, 14 July 2022		
Time	Title	Speaker
2000	Session Chair: Reidun Twarock (University of York)	
2000–2050	Some shape based explorations and manipulations of biomolecules	Chandra Verma A*STAR, Singapore
2050–2140	Topological and algebraic models for studying DNA self-assembly	Nataša Jonoska University of South Florida, USA
2140–2200	<i>Break</i>	

Thursday, 14 July 2022		
Time	Title	Speaker
2200–2250	Virus Structure and Function Through the Lens of Viral Tiling Theory: Novel Opportunities for Antiviral Therapy and Virus Nanotechnology	Reidun Twarock University of York, USA
2250–2340	Modeling knotted proteins with tangles	Isabel Darcy University of Iowa, USA

Friday, 15 July 2022		
Time	Title	Speaker
2000	Session Chair: Andrei Yu. Vesnin (Novosibirsk State University)	
2000–2050	Topological Indices of Fullerenes	Andrei Yu. Vesnin Novosibirsk State University, Russia
2050–2140	Topological and geometrical characterization of three-dimensional porous media	Iskander Taimanov Novosibirsk State University, Russia
2140–2200	<i>Break</i>	
2200–2250	Extremal event graphs: A stable tool for analyzing noisy time series data	Tomas Gedeon Montana State University, USA
2250–2340	Topological Polymers and Random Embeddings of Graphs.	Jason Cantarella University of Georgia, USA