

# DAY 1

December 13, 2021, (Beijing Time)

December 12, 2021, (US Central Time)

Beijing Time	US Central Time	Session Chair: John Z.H. Zhang, Shenzhen Institute of Advanced Technology, China
8:30 – 8:50 AM	6:30 – 6:50 PM	<b>Zoom Registration</b>
8:50 – 8:55 AM	6:50 – 6:55 PM	<b>Welcoming Remark</b> Stephen Shing-Toung Yau, Tsinghua University, China
8:55 – 9:25 AM	6:55 – 7:25 PM	<b>Tamar Schlick</b> , New York University, USA The complex conformational landscape of the SARS-CoV-2 Frameshifting RNA element
9:30 – 9:55 AM	7:30 – 7:55 PM	<b>Weihua Geng</b> , Southern Methodist University, USA A Cartesian FMM-accelerated Galerkin boundary integral Poisson-Boltzmann solver
10:00 – 10:25 AM	8:00 – 8:25 PM	<b>Xiaoqin Zou</b> , University of Missouri - Columbia, USA New strategies to predict protein-peptide interactions
10:30 – 10:55 AM	8:30 – 8:55 PM	<b>Huan-Xiang Zhou</b> , University of Illinois at Chicago, USA Local interactions and transient secondary structures govern backbone dynamics of intrinsically disordered proteins
11:00 – 11:25 AM	9:00 – 9:25 PM	<b>Lin Li</b> , University of Texas at El Paso, USA Developing and applying computational approach to investigate the viral structures
11:30 – 11:55 AM	9:30 – 9:55 PM	<b>Wenrui Hao</b> , Penn State University, USA Computational models of cardiovascular disease

# DAY 2

December 14, 2021, (Beijing Time)

December 13, 2021, (US Central Time)

Beijing Time	US Central Time	Session Chair: Jie Liang, University of Illinois at Chicago, USA
8:50 – 9:00 AM	6:50 – 7:00 PM	<b>Zoom Registration</b>
9:00 – 9:25 AM	7:00 – 7:25 PM	<b>Jie Liang</b> , University of Illinois at Chicago, USA Probability landscapes and global flow maps of discrete flux of stochastic reaction networks: exact construction, computation, and topological analysis
9:30 – 9:55 AM	7:30 – 7:55 PM	<b>Qi Wu</b> , Institute of Microbiology, CAS, China Using Fourier transform to connect response of the trait and the fitness to natural selection
10:00 – 10:25 AM	8:00 – 8:25 PM	<b>Dongqing Wei</b> , Shanghai Jiaotong University, China AIDD and drug candidates by super-computing
10:30 – 10:55 AM	8:30 – 8:55 PM	<b>Zixuan Cang</b> , North Carolina State University, USA Mapping cell-cell communications in spatial transcriptomics data
11:00 – 11:25 AM	9:00 – 9:25 PM	<b>Xi Chen</b> , Xi'an University of Finance and Economics, China Gaussian and Non-Gaussian Colored Noise Induced Escape in a Tumor-Immune Model
11:30 – 11:55 AM	9:30 – 9:55 PM	<b>Rui Dong</b> , Tsinghua University & BIMSA, China Full chromosomal relationships between populations and the origin of humans

# DAY 3

December 15, 2021, (Beijing Time)

December 14, 2021, (US Central Time)

Beijing Time	US Central Time	Session Chair: Alexey Onufriev, Virginia Tech, USA
8:50 – 9:00 AM	6:50 – 7:00 PM	<b>Zoom Registration</b>
9:00 – 9:25 AM	7:00 – 7:25 PM	<b>John Z.H. Zhang</b> , Shenzhen Institute of Advanced Technology, China Structure and interaction of protein-ligand complex
9:30 – 9:55 AM	7:30 – 7:55 PM	<b>Alexey Onufriev</b> , Virginia Tech, USA The Mathematics of Polymer Deformation: Energy Convex Hull Theory
10:00 – 10:25 AM	8:00 – 8:25 PM	<b>Jian Jiang</b> , Wuhan Textile University, China Geometric Graph Learning for Toxicity Prediction
10:30 – 10:55 AM	8:30 – 8:55 PM	<b>Kelin Xia</b> , Nanyang Technological University, Singapore Neighborhood complex based machine learning (NCML) models for drug design
11:00 – 11:25 AM	9:00 – 9:25 PM	<b>Duc Nguyen</b> , University of Kentucky, USA Mathematical-based graph neural network for drug design
11:30 – 11:55 AM	9:30 – 9:55 PM	<b>Yongcheng Zhou</b> , Colorado State University, USA Membrane Pore formation and dual phase field modeling

# DAY 4

December 16, 2021, (Beijing Time)

December 15, 2021, (US Central Time)

Beijing Time	US Central Time	Session Chair: Shi-Jie Chen, University of Missouri, USA
8:20 – 8:30 AM	6:20 – 6:30 PM	<b>Zoom Registration</b>
8:30 – 8:55 AM	6:30 – 6:55 PM	<b>Dmytro Kozakov</b> , Stony Brook University, USA TBA
9:00 – 9:25 AM	7:00 – 7:25 PM	<b>Guowei Wei</b> , Michigan State University, USA Forecasting vaccine-breakthrough SARS-CoV-2 variants
9:30 – 9:55 AM	7:30 – 7:55 PM	<b>Shi-Jie Chen</b> , University of Missouri, USA MgNet: Decoding RNA-metal ion interactions using a deep learning graphical convolutional neural network
10:00 – 10:25 AM	8:00 – 8:25 PM	<b>Ya Jia</b> , Central China Normal University, China A mathematical model for multiple phenotypic states of breast cancer cell
10:30 – 10:55 AM	8:30 – 8:55 PM	<b>Zhiliang Xu</b> , University of Notre Dame, USA Mathematical modeling of blood clotting and cell motion
11:00 – 11:25 AM	9:00 – 9:25 PM	<b>Jinzhi Lei</b> , Tiangong University, China Individual cell-based modeling of tumor cell plasticity-induced immune escape after CAR-T therapy
11:30 – 11:55 AM	9:30 – 9:55 PM	<b>Jiali Gao</b> , University of Minnesota, USA Multistate density functional theory as a matrix functional of densities for excited states