7th Symposium on Biophysics Postgraduate Research in Hong Kong

Event Schedule

Date: Dec 16-18, 2024

Program at a glance

Time/Date	16-Dec-24	17-Dec-24	18-Dec-24
Morning	Arriving	Registration	Safe trip back to home
		Opening session & Picture taking	
		Plenary & Invited speech	
Noon		Lunch	
Afternoon		Students & Postdocs' Presentation	
		Invited Speech	
		Awarding & Closing	

Technical Program

	Morning Session	
8:45 – 12:30	Registration	
9:15 – 9:25	Opening Speech by Prof. Jian Lu, Dean of CENG	
9:25 – 10:10	Plenary Talk (Chair: Prof. Defang Ouyang)	
9:25 – 10:10	**Jianhua Xing**	University of Pittsburgh
	Complex Biology, Simple Physics ----Studying Biological Physics in the Big Data Era	
10:10 – 11:00	Invited Talk (Chair: Prof. Defang Ouyang)	
10:10 – 10:35	**Yanting Wang**	Institute of Theoretical Physics, CAS
	Moderate Point: Balanced Entropy and Enthalpy Contributions in Soft Matter	
10:35 – 11:00	**Yi Wang**	The Chinese University of Hong Kong
	Exploring Plant Enzyme Conformations and Dynamics via MD Simulations	
11:00 – 11:15	Tea Break	
11:15 –12:30	Invited Talk (Chair: Prof. Jhih-Wei Chu)	
11:15 – 11:40	**Jian Zhou**	South China University of Technology
	Molecular Aspects of Proteins at Interfaces	
11:40 – 12:05	**Weikang Wang**	Institute of Theoretical Physics, CAS
	Geometric Quantification of Cell Phenotype Transition Manifolds with Information Geometry	
12:05 – 12:30	**Haibing Su**	Hong Kong University of Science and Technology
	Navigating Bio-Systems Through a Deep Learnt Lens-Scape of Multiscale Analytics	
12:30 – 2:00	Lunch	
	Afternoon Session	
2:00 – 3:40	Students and Postdocs' Presentations (Chair: Kevin Chun Chan)	

2:00 – 2:20	**Ruijian Zhu**	Institute of Theoretical Physics, CAS
	Phase Behavior of Two-Dimensional Model System	
2:20 – 2:40	**Changxiong Huang**	City University of Hong Kong
	Molecular Dynamics Simulations of Nanoslit Sensing in Biomolecular Detection	
2:40 – 3:00	**Cibo Feng**	Hong Kong University of Science &Technology (Guangzhou)
	Hybrid Models Offer Insights into the Relationships Among the Structures, Dynamics, and Functions of Chromosomes	
3:00 – 3:20	**Muhammad Hasan**	Hong Kong University of Science and Technology
	Deciphering Temporal Mutation Patterns in the Spike Glycoprotein: Illuminating Evolutionary Trajectories with the deLemus Platform	
3:20 – 3:40	**Tianjie Li**	The Chinese University of Hong Kong
	Exploring the Role of Transient Interactions in Modulating the Affinity of NF-κB Transcription Factor Rela for DNA Through MD Simulations and Machine Learning	
3:40 – 3:55	Tea Break	
3:55 – 5:35	Invited Talk (Chair: Prof. Haibin Su)	
3:55 – 4:20	**Jhih-Wei Chu**	National Yang Ming Chiao Tung University
	Physics-Based Machine Learning for the Mechanism of Nucleic Acid and Protein Dynamics	
4:20 – 4:45	**Wenjin Li**	Shenzhen University
	Reaction Coordinate Identification and Free Energy Decomposition Analysis from Transition Path Ensemble	
4:45 – 5:10	**Kevin Chun Chan**	Xi'an Jiaotong-Liverpool University
	Antigenic Mimicry in Cross-reactive Recognition through Peptide-MHC Dynamics	
5:10 – 5:35	**Defang Ouyang**	University of Macau
	Computational Pharmaceutics - A New Paradigm of Drug Delivery	
5:35 – 5:45	Awarding of Best Presenters	

Complex Biology, Simple Physics ----Studying Biological Physics in The Big Data Era

Jianhua Xing

Department of Computational and Systems Biology, University of Pittsburgh

Abstract:

One main aim of biological physics is to unravel simple physics principles underlying seemingly complex biological processes. Now we are at a big data age. How do the data and the trend of machine learning/AI change or not change biological physics studies?

The importance of using physical intuition to guess the answer has been repetitively stated by many prominent physicists such as Einstein and Feynman. I would like to argue that physical intuition has guided my research bother before (e.g., mechanism of the bacterial flagellar motor, PNAS 2006, olfactory receptor selection, PNAS 2016) and at the big data era. Here I will focus on our recent study on chromosome folding, a fundamental process in cell biology. Nature has evolved a remarkably robust mechanism to fold 46 human chromosomes (with up to ~10^8 monomers and a total length ~ 2 meters) into segregated territories within a nucleus with size ~ 10 microns or less in a few minutes. People have estimated that it would take ~ 1000 years for a random search. The mechanism must work for all the cell types including cancer cells, against distinct cell type-specific chromosome structure and function requirements, unavoidable stochasticity during the folding process and mutations, otherwise cells would not survive. The secret for achieving this mission impossible hides in public domain (HiC and DNA MERFISH) data, but finding it requires seeing the data through the lens of physics.

Einstein stressed that it is more important to know how to formulate a problem than how to solve it. I will share my experience on reconstructing the governing equations of cellular processes. Physics understanding of a process typically ends at mathematical description. While one can directly apply Newton's equations, Schrodinger's equations, and related formulation to molecular systems, how to write down the equations for cell state change? Our previous publications (Sci Adv 2020, eLife 2022, Cell 2022) provide a general data-driven framework for both cellular kinematics and dynamics. I will present our new efforts and examples of applications, with the long-term goal of constructing virtual cell models parallel to molecular force fields as well as simple models revealing essential physics.

Moderate Point: Balanced Entropy and Enthalpy Contributions in Soft Matter

Yanting Wang[1,2]

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Abstract:

Various soft materials share some common features, such as significant entropic effect, large fluctuations, sensitivity to thermal conditions, and mesoscopic characteristic temporal and spatial scales [1]. Until now, no quantitative definitions have yet been provided for soft matter, and the intrinsic mechanisms leading to their common features are unclear. In this talk, with the aid of an appropriately chosen order parameter, I will define a “moderate point” [2], at which a thermodynamic system has as balanced as possible entropy and enthalpy contributions among its substates. The order parameter fluctuation, the associated response function, and the time and spatial correlation functions all maximize around the moderate point, which explains the characteristics of soft matter mentioned at the beginning. The relation between the moderate point and the so-called “Widom line” [3] as well as a primitive application of this theory to biomachines will also be discussed.

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Exploring plant enzyme conformations and dynamics via MD simulations

Yi Wang

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Abstract:

Molecular dynamics (MD) simulations have been widely adopted to complement experimental techniques in exploring the structures, dynamics and functions of biological macromolecules. In this talk I will discuss my group's work employing MD simulations to probe the structures and dynamics of several plant or fungal enzymes, including the hydroxycinnamoyltransferase (HCT), the aromatic amino acid decarboxylase (AAAD) and the isochorismoyl-glutamate pyruvoyl-glutamate lyase (IPGL). Common to these diverse systems is the critical role played by conformational dynamics, rather than static structural components alone, in mediating the unique function of each protein. I will highlight how their dynamics captured by MD have provided mechanistic insights into the substrate recognition as well as reaction mechanism of these enzymes.

Molecular Aspects of Proteins at Interfaces

Jian Zhou

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Abstract:

The protein orientation and conformation on nano-material surfaces were investigated by multiscale simulations. Based on a coarse-grained protein model, Parallel tempering Monte Carlo algorithm was developed to identify the most favorable adsorption orientation; then all-atom molecular dynamics simulations were applied to further optimize the protein orientation and to investigate the protein conformation change. Effects of surface charge density and sign, and solution ionic strength were examined. Simulation results show that van der Waals and electrostatic interactions codetermine the orientation of adsorbed proteins. The electric dipole and hydrophobic dipole of adsorbed proteins play important roles in determining the protein orientation on charged and hydrophobic surfaces. These concepts are also extened to study the protein orientation and conformation on oil-water interfaces.

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Geometric Quantification of Cell Phenotype Transition Manifolds with Information Geometry

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Abstract:

Cell phenotype transition (CPT) plays a pivotal role in various biological processes like development. Recent advancements in single-cell sequencing techniques have uncovered that cell transition dynamics during development are confined on low-dimensional manifolds. However, existing methods are inadequate for directly quantifying the manifolds from experimental data. Here we present SCIM (single cell information manifolds), a novel geometry-guided method to quantify the CPT manifolds using information geometry. In particular, we convert single cells' high-dimensional gene vectors into probability distributions via Gaussian embedding. The Fisher metric is naturally defined in this embedding space. With the transformed Gaussian distributions, we calculate the coarse Ricci curvature of each single cell. Our analyses reveal that the cells with low curvature are associated with critical transitions. To further examine the invariant characteristics of the manifolds of CPT, we compute the information velocity of each single cell based on RNA velocity. Remarkably, the regions with high information velocity correspond with the low curvature regions, indicating that the geometry can guide the dynamics of single cells on the manifolds. The proposed method not only unveils the invariant characteristics of the CPT manifolds, but also establishes a generic approach for quantifying the intricate dynamics on the CPT manifolds.

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Navigating Bio-Systems Through a Deep Learnt Lens-Scape of Multiscale Analytics

Haibin Su

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Abstract:

Multiparadigm methods to span the scales from atomic dynamics at enzymic reaction centres to practical issues of cells are enabling first principles quantitative explanatory of biological systems with intriguing functions. Bottom-up integration is based on the notions of up-scaling strategy, while top-down effects can be accounted for in terms of effective constraints and inputs. Biological systems are essentially characterized by their evolutionary history. A multiscale scheme is established to unravel the architecture of living systems and their regulation. Recent results ranging from ribosomal peptidyl transferase reaction to cell growth, from F1-ATPase rotation to complex evolutionary landscape of spike glycoprotein in SARS-CoV-2 will be presented.

Physics-Based Machine Learning for the Mechanism of Nucleic Acid and Protein Dynamics

Jhih-Wei Chu (朱智瑋)

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Abstract:

Biomolecules such as protein and nucleic acids carry specific functional properties for carrying out intricate biological processes. A key question is how do such behaviors arrive from the sequence composition and chemical details. Compelling experimental evidence indicates that mechanical properties are essential in the sequence-structure-dynamics-function relationship, but the articulation of which, particularly at the chemical moiety level, remains elusive. In this talk, our development of structure-mechanics statistical learning (SMSL) framework that integrates all-atom molecular dynamics simulations, machine learning, and graph theory is discussed. Findings enabled by this approach include the mechanical relay system in protein allostery, functional conformational changes, and mechanical codes in transcription regulation.

Reaction Coordinate Identification and Free Energy Decomposition Analysis from Transition Path Ensemble

Wenjin Li

Institute for Advanced Study, Shenzhen University

Abstract:

The transition path ensemble (TPE) is a collection of reactive trajectories, all of which largely keep going forward along the transition channel from the reactant state to the product one, and is believed to possess the information necessary for the identification of reaction coordinates. Here, equipartition terms and flux maximization are proposed for the first time for reaction coordinate identification from TPE and the obtained reaction coordinate is well consistent with an ideal reaction coordinate (the committor) [1,2]. In addition, the relationship between flux maximization and the transition path theory is established [3].

On the other hand, free energy decomposition can be used to estimate the contributions from different parts of a system in the transition from one metastable state to the other, which is very useful in mechanistic studies. Typical examples of existing methods are free energy perturbation, thermodynamic integration, and the MM/PB(GB)SA approach. They have their advantages and disadvantages in terms of speed and accuracy. A fast and accurate method is still missing. Here, solutions based on TPE are proposed. Firstly, free energy decomposition along a one-dimensional reaction coordinate is established based on flux-weighted ensemble average over non-equilibrium path ensembles such as TPE and its analogues [4]. Secondly, the approach is applied to resolve the interaction network between opsin and retinal at the residue-wise level [5]. Finally, the approach is extended to cases of multi-dimensional reaction coordinates [6].

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Antigenic Mimicry in Cross-reactive Recognition through Peptide-MHC Dynamics

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Abstract:

The antigen presentation pathway, a key component of the immune response, involves cells presenting intracellular antigenic information to our immune system. Computational modeling of complex biological systems, particularly membrane proteins that present the antigenic peptides, provides valuable insights into these processes. This study investigates the foundation of cross-reactive immunity, where dissimilar where disparate antigenic peptides can trigger similar immune responses. We focus on how antigens associated with class I Major Histocompatibility Complex (MHC) proteins activate specific T-cell subsets, proposing structural mimicry as a key mechanism. Through molecular simulations, we elucidate dynamic aspects of peptide-MHC complexes essential for T-cell receptor (TCR) recognition, enabling precise T-cell activation. Our results demonstrate a direct correlation between the peptides' exposed side chains and their anchor points, showing that different antigens can form structurally similar peptide-MHC surfaces through conformational shifts. This structural similarity allows TCRs to detect changes in peptide anchors, highlighting an allosteric binding mechanism. These findings underscore the significance of surface embedding in peptide-MHC complexes for immune recognition. Furthermore, incorporating these dynamic properties into machine learning models may enhance the prediction of physiological functions, offering promising avenues for the development of more targeted and individualized immunotherapies.

Computational Pharmaceutics - A New Paradigm of Drug Delivery

Defang Ouyang

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Abstract:

In recent decades, the fields of pharmaceutics and drug delivery have become increasingly vital in the pharmaceutical industry, driven by the longer timelines, higher costs, and reduced productivity associated with new molecular entities (NMEs). However, the current formulation development process still depends heavily on traditional trial-and-error methods, which can be time-consuming, expensive, and unpredictable.

Over the past ten years, the rapid advancement of computing power and algorithms has led to the emergence of a new discipline known as “computational pharmaceutics.”[1-2] This field integrates big data, artificial intelligence, and multi-scale modeling techniques into pharmaceutics, presenting significant opportunities to transform drug delivery practices. In this presentation, two examples—solid dispersion and mRNA lipid nanoparticles—will illustrate the application of various computational tools in drug delivery. Computational pharmaceutics offers pharmaceutical scientists multi-scale perspectives, uncovering physical, chemical, mathematical, and data-driven insights across pre-formulation studies, formulation screening, in vivo predictions in the human body, and precision medicine in clinical settings.

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Phase Behavior of Two-Dimensional Model System

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Abstract:

Two-dimensional (2D) systems have attracted significant interests in condensed matter physics due to their novel physical properties and diverse applications, for which comprehensive understandings on phase behaviors of 2D systems are necessary. Theoretically, the so-called 2D crystals have only quasi-long-range translational orders along with long-range bond-orientational orders at finite temperatures. They melt into the liquid state via one of the following three pathways with possible participation of an intermediate phase called hexatic [1]: the KTHNY theory, hard-disk-like behaviour, or regular solid-liquid phase transition.

Benefiting from the fast development of experimental and simulation techniques, extensive research have been performed and achieved comprehensive understandings for 2D systems on both the enthalpy-limited (interactive point-like particles) case and entropy-limited (hard polygons) case. However, these studied systems are still insufficient to understand real 2D molecular systems containing compatible entropy and enthalpy effects. We investigate by molecular dynamics simulation phase stabilities of 2D ball-stick polygons, serving as simplified models for molecular systems [2]. Below the melting temperature T_m, we identify a critical edge number n_c = 4, at which a distorted square lattice emerges; when $n < n_c$, the triangular system stabilizes at a spin-ice-like glassy state; when $n > n_c$, the polygons stabilize at crystalline states. Moreover, in the crystalline state, T_m is higher for polygons with more edges at higher pressures but exhibits a crossover for hexagon and octagon at low pressures. A theoretical framework considers the competition between entropy and enthalpy is proposed to provide a comprehensive understanding of our results, which is anticipated to facilitate the design of 2D materials.

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Molecular Dynamics Simulations of Nanoslit Sensing in Biomolecular Detection

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Abstract:

Nanopore sequencing is a single-molecule sensing technique that offers several advantages, including long readability, high efficiency, and being amplification-free and label-free. The use of nanopores based on two-dimensional materials (2DM) holds the promise of achieving single-base sensing resolution. However, two main challenges need to be addressed to make 2DM nanopore sequencing practical: controlling the translocation speed of biomolecules and detecting distinguishable signals of different building blocks. Aided by molecular dynamics simulations, the processes of nanopore sequencing are studied and some solutions are provided to overcome these challenges. Two sensing strategies are put forward by utilizing the in-plane graphene/hexagonal boron nitride heterostructures. The nanopore with slit shapes are applied and the two strategies are named trans-slit and cross-slit sensing, respectively. First, the factors affecting molecular transportation through nanoslits are presented from dynamic and thermodynamic points of view. Then, the detecting strategies of 2DM nanopore sensing are presented on discriminating DNA base types. Last, cross-nanoslit sensing is also applied to determine the protein lengths. By addressing these challenges and presenting our theoretical findings, this research contributes to the development of more efficient and accurate DNA sequencing methods, as well as explores the potential of nanopore sensing in other areas of biological research.

References

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Hybrid Models Offer Insights Into the Relationships Among the Structures, Dynamics, and Functions of Chromosomes

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Abstract:

Understanding the mechanisms of cell-fate decision-making in cellular development is pivotal for advancing regenerative medicine and addressing neurodegenerative diseases. Cell-fate decision-making is controlled by gene expression networks, which are in turn influenced by the three-dimensional chromosome structures. During cell-fate decision-making processes, chromosomes progressively adapt their structures to accommodate necessary gene expressions. However, understanding the pathways of chromosome structural dynamics during these transitions remains a significant challenge. In this study, we utilized data-driven coarse-grained molecular dynamics simulations and a physics-based non-equilibrium landscape-switching model [1] to quantify chromosome structural dynamics during cell-state transition processes, including differentiation, reprogramming, transdifferentiation, [2,3,4] and cancerogenesis [4]. We quantified the large-scale chromosome structural reorganization pathways during these transitions, and clarified the underlying functional characteristics. Notably, we observed nonmonotonic behaviors in transdifferentiation processes and over-dedifferentiation tendencies in reprogramming processes, from a chromosome structural perspective. Additionally, the chromosome structural dynamical pathways at the scale of topologically associating domains (TADs) exhibited little overlap between forward and reverse directions, in contrast to the ones at the long-range regions, indicating different mechanisms governing these structures. Our study provides a theoretical exploration of cell-fate decision-making from a chromosome structural perspective, offering molecular-level insights into complex cell-state transition processes.

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Deciphering Temporal Mutation Patterns in the Spike Glycoprotein: Illuminating Evolutionary Trajectories with the deLemus Platform

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Abstract:

Throughout the ongoing COVID-19 pandemic caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2)[1], the virus has undergone continuous genomic evolution, leading to the emergence of numerous variants characterized by increased transmissibility and the ability to evade immune responses[2, 3]. The spike glycoprotein of SARSCoV-2, a critical factor in infection and the primary target for antibodies, experiences mutations that significantly influence its evolutionary trajectory.

In this study, we presented a comprehensive analysis of the evolving mutations within the spike protein of SARS-CoV-2. Through the examination of emerging variants, we observe a progressive increase in the effective mutation rate over time. Our investigation delves into the scaling behaviors of the spike glycoprotein, pivotal for understanding the emergence of novel variants carrying multiple mutations. The gradient of mutation distribution presents an early indicator of forthcoming outbreaks, signaling the appearance of new variants. Analysis of amino acid polymorphisms highlighted the virus's inclination for diversification. Additionally, we introduce LMCM (Leading Mutations by Composite Metric), a method that effectively identifies a set of leading mutations evolving together across different time points. By integrating signals from Tucker decomposition applied to a three-dimensional mutation binary matrix and a pair correlation matrix capturing epistatic effects, LMCM unveils the dynamic spectrum of spike protein mutations. The outlined leading mutations provided by the deLemus platform (https://hbsulab.github.io/deLemus/) shed light on mutation trends over time [4], such as shifts in RBD mutations and the Omicron lineage's enhanced flexibility. As evidenced by molecular dynamics, the enhanced flexbility appears to be influenced by underlying physicochemical alterations within specific domains, notably leading to increased hydrophilicity, charge, and polarity within the NTD loops and the RBM. These findings elucidated the virus's adaptive strategies and mutation dynamics over time, offering valuable insights into its evolving behavior.

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Exploring the Role of Transient Interactions in Modulating the Affinity of NF-κB Transcription Factor Rela for DNA Through MD Simulations and Machine Learning

Tianjie Li, Yi Wang

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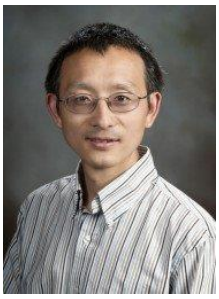
Abstract:

Nuclear factor kappa B (NF-κB) transcription factors are crucial for gene regulation, binding to κB DNA elements characterized by a variable central region flanked by conserved sequences. The RelA homodimer, a commonly expressed NF-κB transcription factor, exhibits varying affinities depending on the central DNA base pair, with A or T providing a tenfold higher affinity than G or C. However, their nearly identical crystal structures offer limited insights into the mechanisms behind these affinity variations. Our research employed extensive molecular dynamics (MD) simulations and machine learning to identify two critical residues, R187 and R124, in RelA and to clarify their unique dynamic behaviors. R187 affects base contacts by interacting with residues in the major groove through different transient states, whereas R124 enhances interactions by promoting transient insertion into the minor groove of A-κB sequences compared to G-κB. These residues demonstrate selective interactions that create a complex interplay among DNA-interacting residues, which was confirmed through mutagenesis studies. Our findings illuminate the intricate mechanisms that govern NF-κB's selective binding to κB DNA, highlighting the significance of MD simulations in revealing the dynamic nature of transcription factor-DNA interactions.

References

[1] Tianjie Li, Shandy Shahabi, Tapan Biswas, Oleg V Tsodikov, Wenfei Pan, De-Bin Huang, Vivien Ya-Fan Wang, Yi Wang, and Gourisankar Ghosh. Transient interactions modulate the affinity of NF-κB transcription factors for DNA. Proceedings of the National Academy of Sciences. 121.23 (2024), pp. e2405555121. DOI: 10.1073/pnas.2405555121.

Jianhua Xing University of Pittsburgh



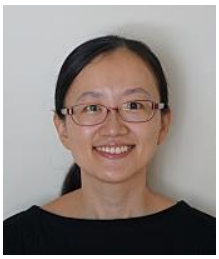
Prof. Jianhua Xing received B.S. in Chemistry from Peking University, M.S. in Chemical Physics from University of Minnesota, and PhD in Theoretical Chemistry from UC Berkeley. After being a postdoc researcher in theoretical biophysics at UC Berkeley and an independent fellow at Lawrence Livermore National Laboratory, he assumed his first faculty position at Virginia Tech, then moved to University of Pittsburgh in 2015. Currently Dr Xing is a professor in the Computational and Systems Biology Department, School of Medicine, and an affiliated faculty member of Department of Physics and Astronomy, University of Pittsburgh. He is also an affiliated member of University of Pittsburgh Hillman Cancer Center. He is an editorial board member of Biophysical Journal.

Dr Xing's research uses statistical and chemical physics, dynamical systems theory, mathematical/computational modelling in combination with quantitative measurements to study the dynamics and mechanics of biological processes. In recent years one major research direction in his lab is to develop an integrated theoretical/computational-experimental framework of reconstructing governing equations of cellular processes (e.g., Sci Adv 2020, eLife 2022, Cell 2022, PRX Life 2024), with the long-term goal of constructing virtual cell models parallel to molecular force fields, and from which developing simple models revealing essential physics for complex systems.

Yanting Wang Institute of Theoretical Physics, CAS

Prof. Yanting Wang is a full professor at the Institute of Theoretical Physics, Chinese Academy of Sciences (ITP-CAS). From 1990-1999, he studied in the Department of Modern Physics, University of Science and Technology of China, and obtained a bachelor's degree in nuclear electronics and a doctorate in nuclear physics. From 1999-2004, he studied at the University of Rochester in the United States and obtained a doctorate in theoretical condensed matter physics. From 2004-2009, he worked as a postdoc in the Department of Chemistry at the University of Utah and at the Idaho National Laboratory of the US, respectively. Since 2009, he has successively served as an associate professor and a full professor at the ITP-CAS, and additionally served as the deputy director of ITP-CAS from 2017 to 2022. His research interests lie in using molecular simulation combined with statistical theory to comprehensively study the structural and dynamic properties, phase transitions and phase behaviors of soft matter and biomolecular systems, such as nanometals, complex liquids, polypeptides and proteins. So far, he has published more than 90 peer-review papers, which have been cited more than 5,000 times with an h-index of 31.

Yi Wang The Chinese University of Hong Kong



Prof. Yi Wang is an associate professor in the Physics department of the Chinese University of Hong Kong. Her group works on molecular dynamics (MD) simulations of biomolecules, with research topics spanning all four categories of biological macromolecules, namely, proteins, lipids, carbohydrates as well as nucleic acids. Recent work from Prof. Wang's lab includes the calculation of free energy barriers against drug or drug-like molecules' permeation, the characterization of nanoparticle-membrane interactions, the dynamics of plant/fungal enzymes as well as the kinetics of supramolecular hydrogels.

Jian Zhou South China University of Technology

Prof. Jian ZHOU obtained his Ph.D. degree (Chem. Eng.) at NanJing University of Technology, China, in 1998. After that, he had postdoc researches at Beijing University of Chemical Technology, Univ. of Washington and Univ. of Utah. Since 2006, he has been employed as a full professor in the School of Chemistry and Chemical Engineering at South China University of Technology.

He has published 180+ SCI-indexed papers at international journals. He won the New Century Talents Award and Fok Ying Tung Young Faculty Award. He is Elsevier Highly Cited Chinese Researcher since 2020. His main research field is multiscle modeling and simulation of complex systems, such as protein adsorption, responsive polymers etc.

Weikang Wang Institute of Theoretical Physics, CAS

Prof. Wang Weikang is an associate researcher at the Institute of Theoretical Physics, Chinese Academy of Sciences. He obtained his bachelor's and doctoral degrees from the School of Physics at Peking University in 2009 and 2015, respectively. Subsequently, he conducted postdoctoral research in the Department of Computational and Systems Biology at the University of Pittsburgh. His research areas include biophysics, computational and systems biology. His current research interests involve the dynamics of cell state transitions, the statistical physical properties of gene regulatory networks and neural networks, and the development of machine learning methods to analyze gene regulatory networks.

Haibing Su Hong Kong University of Science and Technology

Prof. Haibin Su is a computation scientist. He received his Ph.D. from The State University of New York at Stony Brook, then went to Caltech for a 3-yr PostDoctoral prior to joining Nanyang Technological University. Since 2018, he joined department of chemistry at The Hong Kong University of Science and Technology. His research interest includes development and application of theoretical and computational methods: i.e., quantum-mechanical and classical simulations and modeling of the electronic, structural, energetical, and dynamical properties of chemical and biological systems.

Jhih-Wei Chu National Yang Ming Chiao Tung University

Prof. Jhih-Wei Chu is a distinguished professor and director at the Institute of Bioinformatics and Systems Biology and the Department of Biological Science and Technology at National Yang Ming Chiao Tung University in Hsinchu, Taiwan. He earned his PhD in Chemical Engineering from the Massachusetts Institute of Technology (MIT) in 2004, following his BS and MS degrees from National Taiwan University. His research focuses on protein dynamics, allostery, multiscale modeling, statistical mechanics, and drug discovery.

Professor Chu has received several prestigious honors, including the International Outstanding Junior Scholar Award and the Award for Recruiting Outstanding International Scholars. His recent publications in high-impact journals such as *Chemical Science* and *Nature Chemistry* showcase his innovative work in protein mechanics and DNA motifs. With a commitment to advancing computational biology, his contributions have significant implications for understanding molecular mechanisms and developing therapeutic strategies.

Wenjin Li Shenzhen University

Dr. Wenjin Li is a tenured associate professor who obtained his Ph.D. in Computational Biology from the Shanghai Institute for Biological Studies, Chinese Academy of Sciences, in 2012. He then worked as a postdoctoral researcher at the University of Illinois at Chicago in the United States. In 2017, he joined the Institute for Advanced Studies, Shenzhen University, as a principal investigator (assistant professor), and was promoted to tenured associate professor in 2024. Dr. Li has also stayed as visiting scholar for nearly three years at the Max Planck Institute for Biophysical Chemistry and the Heidelberg Institute for Theoretical Studies in Germany. His main research interests lie in theoretical calculations of biological macromolecules and computer-aided drug discovery, including reaction coordinate identification, energy decomposition along reaction coordinates, and mechanistic studies of protein-small molecule ligands and protein-nucleic acid systems with molecular dynamics simulations. His work has been supported by funds from both National Natural Science Foundation of China and Natural Science Foundation of Guangdong Province, China. He has published over 40 papers in prestigious international journals, such as JACS, JCTC, PCCP, JCP, and JPCA. Dr. Li has been awarded Shenzhen Overseas High Level Talent (Peacock Plan, Level C). He also serves as a Youth Editorial Board Member of Interdisciplinary Sciences: Computational Life Sciences.

Kevin Chun Chan Xi'an Jiaotong-Liverpool University

Dr. Kevin C. Chan received his PhD from City University of Hong Kong in 2017. He finished his postdoctoral training at College of Pharmacy, Ohio State University in 2021. He then returned to China, as a fellow at Shanghai Institute for Advanced Study, Zhejiang University until early 2024. Meanwhile, he was a postdoctoral researcher at the Institute of Quantitative Biology, College of Life Sciences of Zhejiang University and Center for Precision Medicine of Shenzhen Luohu People's Hospital. Recently, he joined Xi'an Jiaotong-Liverpool University as an Assistant Professor.

Since his PhD, Kevin has pursued interdisciplinary research at the interface of molecular simulation, drug discovery and machine learning. His current interests focus on artificial intelligence for biomolecular dynamics (AI4Science), molecular simulation of various complex biomolecular systems including the human immunological synapse, the bacterial membrane protein assembly, the CRISPR genome editing tools, and design of molecular glues for protein machinery. Dr. Chan has published 20+ papers in peer-reviewed journals, including *Nature, Nature Communications, PNAS, JCIM, JPCB* etc. He actively serves in the academic community as a member of *The Protein Society, American Chemical Society (COMP), and Biophysical Society*. He is also a committee member of *The Bioinformatics Society of China*.

Defang Ouyang University of Macau

Prof. Ouyang has a multidisciplinary background in pharmaceutics & computer modelling, with experience in academia and industry. He obtained his bachelor (2000) and master (2005) in pharmaceutics from Shenyang Pharmaceutical University, China. He completed his PhD in pharmacy at The University of Queensland, Australia, in 2010 and progressed directly to his faculty position (Lecturer in Pharmaceutics, PI) at Aston University (UK). From the end of 2014, he moved to the University of Macau.

Since 2011, he has pioneered the integration of multi-scale modelling, artificial intelligence and big data techniques in the field of drug delivery – "**computational pharmaceutics**". He has published 2 books, 5 book chapters, over 100 refereed SCI journal papers, and over 100 invited talks. He held 11 approved patents, which had been used in medicinal products. He edited the first book <Computational Pharmaceutics - the application of molecular modelling in drug delivery> (John Wiley & Sons Inc., 2015) in this research area. He serves as the associate editor of <Drug Delivery and Translational Research>, editorial board/scientific advisor of <Asian Journal of Pharmaceutical Sciences>, <Pharmaceutical Research> and <Journal of Pharmaceutical Sciences>. He established the first artificial intelligence (AI)-based formulation platform (FormulationAI). He successfully trained 6 PhD and 30 master students.

His research focused on computational pharmaceutics, including:

- Artificial intelligence (AI) of pharmaceutical formulations: to build the database of pharmaceutical formulations and predict pharmaceutical formulations by machine learning approaches.
- Multi-scale modelling in drug delivery: to integrate quantum mechanics (QM), molecular dynamics (MD) and physiologically based pharmacokinetic (PBPK) modelling into drug delivery systems;
- Pharmacoinformatics: big data analysis of pharmaceutical information from the literature, patent, clinical trial and marketed products.

Ruijian Zhu Institute of Theoretical Physics, CAS

Mr. Ruijian Zhu is a second-year graduate student at the Institute of Theoretical Physics, Chinese Academy of Sciences (ITP-CAS), under the supervision of Prof. Yanting Wang. He has been awarded the National Scholarship for Master's Students in 2024. Prior to this, he obtained a Bachelor of Science degree from University of Chinese Academy of Sciences (UCAS), where he was honored as an Excellent Graduate of Beijing and received the Outstanding Undergraduate Thesis Award. His current research is aimed at understanding the phase behavior in soft matter system through molecular simulation.

Cibo Feng Hong Kong University of Science &Technology (Guangzhou)

Mr. Cibo Feng is a second year Ph.D. student from the group of Assistant Professor Xiakun Chu, the Advanced Material Thrust, the Hong Kong University of Science and Technology (Guangzhou). He graduated with a bachelor's degree in physics from Jilin University, His research interest focuses on the biophysics mechanism analysis using coarse-grained molecular dynamics simulation and on the exploration of the relationship between structure, dynamics and functions of biomacromolecules. He has published two papers in respectively Journal of Molecular Cell Biology and Physical Review Research.

Changxiong Huang City University of Hong Kong

Dr. Changxiong Huang obtained his PhD degree from CityUHK, where he was supervised by Prof. Jun Fan. Currently, he is working as a postdoctoral researcher in the Department of Materials Science and Engineering at CityUHK, under the guidance of Prof. Xiaocheng Zeng. Up to now, as first author and/or co-corresponding author, he has published papers in JPCL, ACS Nano, Nat. Commun, and so on. His research primarily involves the use of molecular dynamics simulations to investigate various nanoscale phenomena and their applications. Some of the key areas of his research include DNA and protein detection using nanopore sensing, molecular transportation within nano-confined volumes, and the self-assembly of molecules in liquid phases.

Muhammad Hasan Hong Kong University of Science and Technology

Dr. Muhammad Hasan is a post-doctoral fellow at The Hong Kong University of Science and Technology (HKUST) in the Theoretical & Computational Chemistry Lab. He earned his Ph.D. in Chemistry from HKUST in 2024. He is a recipient of the prestigious Belt and Road Scholarship and was awarded a silver medal in the National Physics Olympiad.

His research focuses on computational chemistry and the electronic structure of materials, with notable contributions in exploring mutations in SARS-CoV-2 spike glycoproteins. Muhammad Hasan's work has been presented at international conferences and published in reputable journals.

Tianjie Li The Chinese University of Hong Kong

Dr. Tianjie Li is a postdoctoral researcher in Prof. Yi Wang's group at the Chinese University of Hong Kong. He earned his Ph.D. from South China University of Technology. His research focuses on the mechanistic study of biomacromolecules, including enzymes and transcription factors, and the multiscale investigation of biomaterial interfaces through computational models. His work has been published in prestigious journals, including Nature Communications, PNAS, and Advanced Functional Materials.