



北京大学定量生物学中心
CENTER FOR QUANTITATIVE BIOLOGY

Quantitative Biology 2017: Computational and Single-Molecule Biophysics

Friday 23 June 2017 - Monday 26 June 2017

Peking University, China
Programme

Quantitative Biology 2017: Computational and Single-Molecule Biophysics

Host Center for Quantitative Biology (CQB)
Academy for Advanced Interdisciplinary Studies
Peking University
<http://cqb.pku.edu.cn/en/>

Organizers **Computational Biophysics**
Dr. Chen Song (CQB, Peking University)
Single-Molecule Biophysics
Dr. Zhi Qi (CQB, Peking University)

Consultants **Computational Biophysics**
Prof. Luhua Lai (CQB, Peking University)
Prof. Mark S. P. Sansom (Oxford, UK)
Single-Molecule Biophysics
Prof. Ming Li (Institute of Biophysics, CAS)
Prof. Yann Chemla (UIUC, USA)

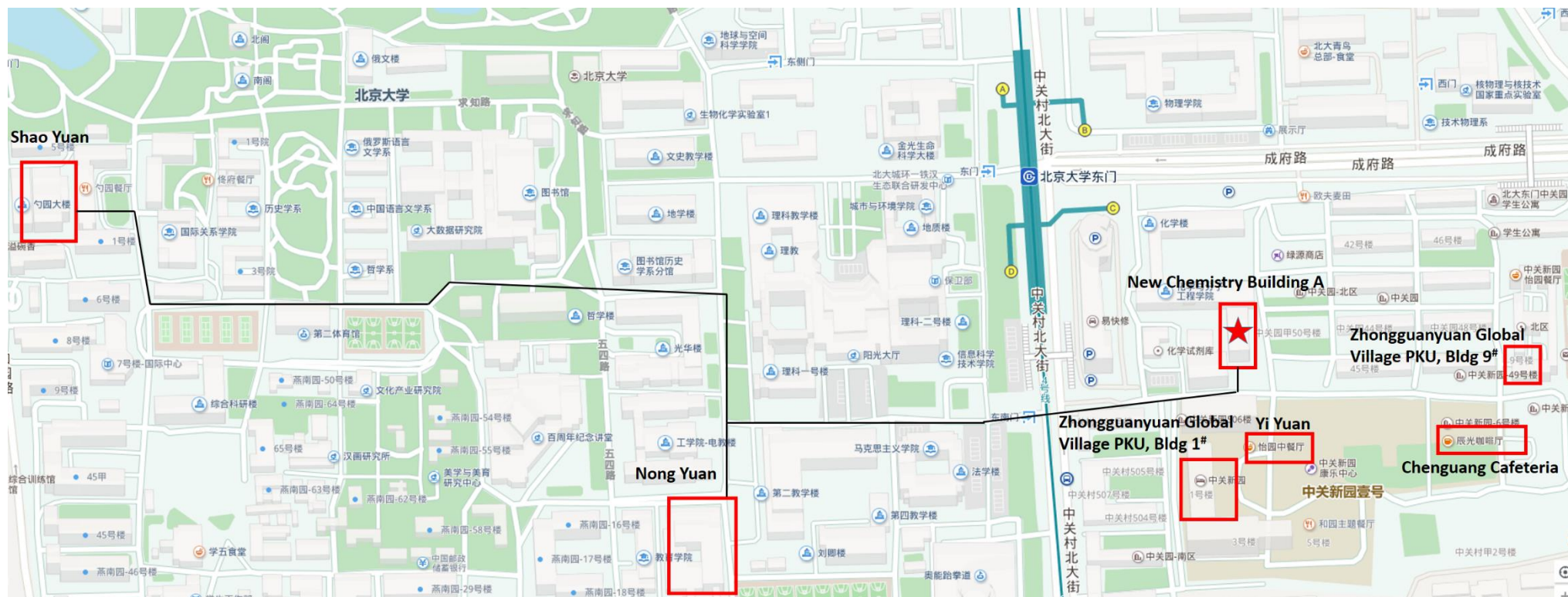
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Venue Address

A204, New Chemistry Building (北京大学化学与分子工程学院新化学楼A204)

Address: 202 Chengfu Road, Haidian District, Beijing, China (北京市海淀区成府路202号)

Website: <http://indico.pku.edu.cn/e/QB2017>



Saturday 24 June 2017

Registratoin - A204, New Chemistry Building (07:00-07:50)

Opening - A204, New Chemistry Building (08:00-08:15)

Talk: Computational Session 1 - A204, New Chemistry Building (24 June 08:15-10:05)

- Conveners: Dr. Song, Chen (Peking University)

time	title	presenter
08:15	Designing Allosteric Ligands to Regulate Protein Function	Prof. LAI, Luhua (Peking University)
08:45	The molecular dynamics of channel permeation and molecular recognition	DE GROOT, Bert (Max Planck Institute for biophysical chemistry)
09:15	Multi-scale modeling of 3-D chromatin structures	GAO, Yiqin (College of Chemistry and Molecular Engineering, and Biodynamics Optical Imaging Center, Peking University)
09:45	Multiscale Modeling of Protein Self-Assembly in the Solution and the Membrane	Prof. LI, Jianing (University of Vermont)

Photo and Tea Break - A207, New Chemistry Building (10:05-10:35)

Talk: Single-Molecule Session 1 - A204, New Chemistry Building (24 June 10:35-12:05)

- Conveners: Dr. Qi, Zhi (Peking University)

time	title	presenter
10:35	Probing protein-nucleic acid dynamics with 'next generation' single-molecule techniques	Prof. CHEMLA, Yann (University of Illinois, Urbana-Champaign, USA)
11:05	Dynamics and regulation of the RAD51 nucleoprotein filament	Prof. SPIES, Maria (University of Iowa, USA)
11:35	Genome-scale biophysical profiling of CRISPR interference	Prof. FINKELSTEIN, Ilya (University of Texas at Austin, USA)

Lunch and Break - Nongyuan 农园 (12:05-13:30)

Talk: Computational Session 2 - A204, New Chemistry Building (24 June 13:30-15:10)

- Conveners: Prof. Li, Jianing (University of Vermont)

time	title	presenter
13:30	Conformational ensemble of intrinsically disordered tau protein: insight into the aggregation mechanism	Prof. WEI, Guanghong (Fudan University)
14:00	Molecular Dynamics Simulations of the E.coli Cell Envelope: capturing the complexity	Prof. KHALID, Syma (University of Southampton)

14:30	Integrative models of complete viruses – Combining Structure, Genomics and Modeling	Dr. HUBER, Roland G (Bioinformatics Institute (BII), Agency for Science Technology and Research (A*STAR))
14:50	Computational Studies on the Function Mechanisms of Two Antimicrobial Peptides	Dr. SONG, Chen (Peking University)

Tea Break - A207, New Chemistry Building (15:10-15:30)

Talk: Single-Molecule Session 2 - A204, New Chemistry Building (24 June 15:30-16:50)

- Conveners: Dr. Chen, Chunlai (Tsinghua University)

time	title	presenter
15:30	High precision single-molecule techniques for molecular biophysics and membrane biophysics	Prof. LI, Ming (Institute of Physics, Chinese Academy of Sciences, China)
16:00	Kinetic analysis of substrate degradation by the proteasome	Prof. LV, Ying (Harvard University, USA)
16:30	Investigating interactions between human RAD52, Replication Protein A, and RAD51 on ssDNA using DNA curtains	MA, Frank (Columbia University Medical Center)

Poster - A204, New Chemistry Building (24 June 16:50-17:50)

Dinner and Break - Nongyuan 农园 (18:00-19:00)

Career Discussion - A205, New Chemistry Building (19:00-20:00)

Poster - A204, New Chemistry Building (24 June 20:00-21:00)

Sunday 25 June 2017

Talk: Single-Molecule Session 3 - A204, New Chemistry Building (25 June 08:00-09:50)

- Conveners: Dr. NIU, HENGYAO (Molecular and Cellular Biochemistry Department, Indiana University Bloomington)

time	title	presenter
08:00	Single-molecule Electron Spin Resonance Spectroscopy and Imaging by diamond sensor	Prof. DU, Jiangfeng (University of Science and Technology of China)
08:30	Cryo-EM study of human RAD51 recombinase filaments during catalysis of DNA-strand exchange	Prof. WANG, Hongwei (Tsinghua University)
09:00	DECIPHERING THE STOCHASTIC KINETICS OF GENE REGULATION	Prof. GOLDING, Ido (Baylor College of Medicine)
09:30	ssDNA Curtains for Studying RPA Binding Mode	Dr. QI, Zhi (Peking University)

Tea Break - A207, New Chemistry Building (09:50-10:10)

Talk: Computational Session 3 - A204, New Chemistry Building (25 June 10:10-12:00)

- Conveners: Prof. Cheng, Shengfeng (Virginia Polytechnic Institute and State University)

time	title	presenter
10:10	Molecular dynamics as a new tool for elucidation of structural basis of kinase regulation by the regulatory domains	Prof. SHAN, Yibing (D. E. Shaw Research/Computational Science Research Center, Beijing)
10:40	Large Scale Molecular Simulation of Nanoparticle-Biomolecule Interactions and their Implications in Nanomedicine	Prof. ZHOU, Ruhong (IBM Research and Columbia University)
11:10	From Molecular Dynamics to Genomic Biology: Constructing Kinetic Network Models to Elucidate Transcriptional Fidelity of RNA Polymerase II	Prof. HUANG, Xuhui (The Hong Kong University of Science and Technology)
11:40	Simulating the conformational change of membrane transporters and channels	Dr. GONG, Haipeng (Tsinghua University)

Lunch and Break - Nongyuan 农园 (12:00-13:30)

Poster - A204, New Chemistry Building (25 June 13:30-14:00)

Talk: Single-Molecule Session 4 - A204, New Chemistry Building (25 June 14:00-15:50)

- Conveners: Prof. Lv, Ying (Harvard University, USA)

time	title	presenter
14:00	The effects of cytosine methylation on general transcription factors	Prof. SU, Xiaodong (BIOPIC, Peking University, China)
14:30	Dynamics and mechanisms of bio-molecules revealed by single molecule FRET	Prof. CHEN, Chunlai (Tsinghua University, China)
15:00	Mechanisms of genomic ribonucleotide removal in yeast	Dr. NIU, HENGYAO (Department of Molecular and Cellular Biochemistry, Indiana University Bloomington)

15:30	Probing Molecules Binding to Unfolded Polyprotein Based on its Elasticity and Refolding	Mr. TANG, Qingnan (Department of Physics, National University of Singapore, Singapore, Singapore)
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Tea Break - A207, New Chemistry Building (15:50-16:10)

Talk: Computational Session 4 - A204, New Chemistry Building (25 June 16:10-17:50)

- Conveners: Prof. Li, Weifeng (Medical School, Soochow University)

time	title	presenter
16:10	Emergence of collective oscillation in cell populations: a nonequilibrium thermodynamic narrative	Prof. TANG, Leihan (Beijing Computational Science Research Center)
16:40	Classification of Proteomes and Protein Sets Based on Their Protein Distributions in Terms of Protein Lengths and Protein Intrinsic Disorder Contents	Prof. GUO, Hong (University of Tennessee Knoxville)
17:10	Structural ensemble of intrinsically disordered protein determined by enhanced sampling and NMR restraints	Dr. DUAN, Mojie (Wuhan Institute of Physics and Mathematics, Chinese Academic of Sciences)
17:30	The entropic effect of disordered linkers in allosteric regulation	Mr. LI, Maodong (Peking University)

Reception - Chenguang Cafeteria 中美新园晨光咖啡厅 (18:00-21:00)

Monday 26 June 2017

Talk: Computational Session 5 - A204, New Chemistry Building (26 June 08:00-09:40)

- Conveners: Dr. Gong, Haipeng (Tsinghua University)

time	title	presenter
08:00	Polarizable force field for cellular membrane lipids and acceleration strategy for MD simulation	Prof. LI, Guohui (Dalian Institute of Chemical Physics, Chinese Academy of Sciences)
08:30	Electronic polarization effects in membrane transport	Prof. NOSKOV, Sergei (University of Calgary)
09:00	Effects of Spermines on Microtubule Conformations	Prof. CHENG, Shengfeng (Virginia Tech)
09:20	Exploring the Biological Effects and Cytotoxicity of Nanomaterials with Computer Simulation	Prof. LI, Weifeng (Medical School, Soochow University)

Tea Break - A207, New Chemistry Building (09:40-10:00)

Talk: Single-Molecule Session 5 - A204, New Chemistry Building (26 June 10:00-11:20)

- Conveners: Ma, Frank (Columbia University Medical Center)

time	title	presenter
10:00	Deciphering Stochastic Transcriptional Regulation at an Endogenous Gene Locus	Dr. XU, Heng (Institute of Natural Sciences, Shanghai Jiao Tong University)
10:30	Incoherent inputs enhance robustness of biological oscillators	Prof. YANG, Qiong (University of Michigan)
11:00	Investigating the mechanism of nuclear transport using a DNA-origami scaffolded artificial nuclear pore complex	Dr. SHEN, Qi (Department of Cell Biology, Yale University School of Medicine; Nanobiology Institute, Yale University)

Award and Closing - A204, New Chemistry Building (11:20-11:40)