JUNHUI PENG, PhD

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EDUCATION

Ph.D. University of Science and Technology of China (USTC) Jul 2017
Computational Biology, School of Life Sciences
Advisor: Dr. Zhiyong Zhang & Dr. Yunyu Shi

B.S. University of Science and Technology of China (USTC) Jun 2012
Biology, School of Life Sciences
Advisor: Dr. Zhiyong Zhang & Dr. Yunyu Shi

RESEARCH EXPERIENCES

Postdoctoral Researcher, Rockefeller University Jul 2019 – present

Advisor: Dr. Li Zhao

- Developed a computational platform to study the origin and evolution of the interactions between sex peptide and sex peptide receptor. This demonstrates how genetic novelty gives rise to novel protein-protein interactions.
- Developed a computational pipeline to identify *Drosophila* specific *de novo* genes and study how genetic novelty gives rise to protein structure novelty.
- Demonstrated how intermolecular interactions drive protein sequence adaptative evolution in *Drosophila melanogaster* by comparative genomics analysis and populational genomics analysis.
- Collaborated with Prof. Hironori Funabiki, Prof. Kivanç Birsoy, and other colleagues in comparative genomic analysis, populational genomics analysis, and computational biology studies.

Postdoctoral Researcher, Hong Kong University of Science and Technology (HKUST) Oct 2017 – Jun 2019

Advisor: Dr. Xuhui Huang

- Applied molecular dynamics simulations to study the dynamics of nucleosome DNA unwrapping.
- Collaborated with Prof. Benzhong Tang and other colleagues in computational biophysics studies.

Graduate studies, University of Science and Technology of China (USTC) Sep 2012 – Jun 2017

School of Life Sciences
Advisor: Dr. Zhiyong Zhang & Dr. Yunyu Shi

- Thesis: The development and application of computational platforms that integrates real world biophysical data to study the structure and dynamics of biomolecules.
- Collaborated with Prof. Ming Lei, Prof. Qingguo Gong, Prof. Congzhao Zhou, and other colleagues in computational biology.

Undergraduate studies, USTC Sep 2011 – Jun 2012

School of Life Sciences
Advisor: Zhiyong Zhang & Yunyu Shi

FUNDING & AWARDS

Shapiro-Silverberg Fund for the Advancement of Translational Research, The Rockefeller University Center for Clinical and Translational Science (RUCCTS) 2024

SMBE Travel Award, Society for Molecular Biology and Evolution 2023

C. H. Li Memorial Scholar Fund Award, Rockefeller University 2021
CAS President Award (Excellence Award), Chinese Academy of Science 2017

PRESENTATIONS

Oral, SMBE Satellite Meeting on De Novo Gene Birth, Texas A&M University, TX Nov 2023
Oral, the 64th Annual Drosophila Research Conference, Chicago, IL Mar 2023
Oral, 2023 New York Area Population Genomics Meeting Jan 2023
Oral, BSVMRKYZ Super-Group Meeting, Rockefeller University, NY Nov 2022
Oral, Pels Family Center Chemical and Structural Biology Retreat, Edith Macy Center, NY Oct 2022
Poster, virtual, the 63rd Annual Drosophila Research Conference Apr 2022
Oral, virtual, the 2nd AsiaEvo Conference Aug 2021
Oral, Chinese Society of Biochemistry and Molecular Biology Conference, Xiamen, China Aug 2014

PUBLICATIONS *(more information at my google scholar profile)*

Postdoctoral research, Rockefeller University

1. Wassing, I. E., Nishiyama, A., Shikimachi, R., Jia, Q., Kikuchi, A., Hiruta, M., Sugimura, K., Hong, X., Chiba, Y., **Peng, J.**, Jenness, C., Nakanishi, M., Zhao, L., Arita, K., Funabiki, H. (2024). CDCA7 is an evolutionarily conserved hemimethylated DNA sensor in eukaryotes. ***Science Advances***, 10(34), 2024
2. **Peng, J.**, Svetec, N., Molina N., Zhao L. *The origin and evolution of the interactions between sex peptide and sex peptide receptor*. ***Mol Biol Evol*** msae065, 2024
3. **Peng, J.**, Zhao, L. *The origin and structural evolution of de novo genes in Drosophila*. ***Nat Commun*** 15, 2024
4. Liu Y., Liu S., Tomar A., Yen F., Unlu G., Ropek N., Weber R., Wang Y., Khan A., Gad M., **Peng J.**, et al. *Autoregulatory control of mitochondrial glutathione homeostasis*. ***Science*** 382, 820-828, 2023
5. Chung, K., Xu, L., Chai, P., **Peng, J.**, Devarkar, S. C., Pyle, A. M. *Structures of a mobile intron retroelement poised to attack its structured DNA target*. ***Science*** 378, 627-634, 2022
6. **Peng, J.**, Svetec, N., Zhao, L. *Intermolecular Interactions Drive Protein Adaptive and Coadaptive Evolution at Both Species and Population Levels*. ***Mol Biol Evol*** msab350, 2022
7. Durkin, S.M., Chakraborty, M., Abrieux, A., Lewald, K.M., Gadau, A., Svetec, N., **Peng, J.**, Kopyto, M., Langer, C.B., Chiu, J.C., et al. *Behavioral and genomic sensory adaptations underlying the pest activity of Drosophila suzukii*. ***Mol Biol Evol*** msab048, 2021

Postdoctoral research, HKUST

8. Pan, C., Liu, C., **Peng, J.**, Ren, P., and Huang, X. *Three-site and five-site fixed-charge water models compatible with AMOEBA force field*. ***J Comput Chem*** 41, 2020
9. Zhang, J., Li, A., Zou, H., **Peng, J.**, Guo, J., Wu, W., Zhang, H., Zhang, J., Gu, X., Xu, W., et al. *A "simple" donor-acceptor AIEgen with multi-stimuli responsive behavior*. ***Mater Horiz*** *7*, 2020
10. Zhang, J., Liu, Q., Wu, W., **Peng, J.**, Zhang, H., Song, F., He, B., Wang, X., Sung, H.H.Y., Chen, M., et al. *Real-Time Monitoring of Hierarchical Self-Assembly and Induction of Circularly Polarized Luminescence from Achiral Luminogens*. ***ACS Nano*** 13, 2019
11. **Peng, J.**, Wang, W., Yu, Y.Q., Gu, H.L., and Huang, X. Clustering algorithms to analyze molecular dynamics simulation trajectories for complex chemical and biological systems. ***Chin J Chem Phys*** 31, 2018

Graduate research, USTC

12. **Peng, J.#**, Yuan, C.#, Hua, X., Zhang, Z*. Molecular mechanism of histone variant H2A.B on stability and assembly of nucleosome and chromatin structures*. *Epigenetics Chromatin* 13, 2020 **(# co-first author**)
13. **Peng, J.#,** Yuan, C.#, Ma, R., Zhang, Z. *Backmapping from Multiresolution Coarse-Grained Models to Atomic Structures of Large Biomolecules by Restrained Molecular Dynamics Simulations Using Bayesian Inference*. ***J Chem Theory Comput*** 15, 2019 **(# co-first author**)
14. Xu, D., Ma, R., Zhang, J., Liu, Z., Wu, B., **Peng, J.**, Zhai, Y., Gong, Q., Shi, Y., Wu, J., et al. *Dynamic Nature of CTCF Tandem 11 Zinc Fingers in Multivalent Recognition of DNA As Revealed by NMR Spectroscopy*. ***J Phys Chem Lett*** 9, 2018
15. Cheng, P.#, **Peng, J.#**, and Zhang, Z. (2017). SAXS-Oriented Ensemble Refinement of Flexible Biomolecules. Biophys J 112, **(# co-first author**)
16. Chen, C., Gu, P., Wu, J., Chen, X., Niu, S., Sun, H., Wu, L., Li, N., **Peng, J.**, Shi, S., et al. *Structural insights into POT1-TPP1 interaction and POT1 C-terminal mutations in human cancer*. ***Nat Commun*** 8, 2017
17. Xu, L., Wang, L., **Peng, J.**, Li, F., Wu, L., Zhang, B., Lv, M., Zhang, J., Gong, Q., Zhang, R., et al. *Insights into the Structure of Dimeric RNA Helicase CsdA and Indispensable Role of Its C-Terminal Regions*. ***Structure*** 25, 2017
18. **Peng, J.**, Zhang, Z. *Unraveling low-resolution structural data of large biomolecules by constructing atomic models with experiment-targeted parallel cascade selection simulations.* ***Sci Rep*** 6, 2016
19. Shao, Z., Yan, W., **Peng, J.**, Zuo, X., Zou, Y., Li, F., Gong, D., Ma, R., Wu, J., Shi, Y., et al. *Crystal structure of tRNA m1G9 methyltransferase Trm10: Insight into the catalytic mechanism and recognition of tRNA substrate*. ***Nucleic Acids Res*** 42, 2014
20. **Peng, J.**, Zhang, Z. Simulating large-scale conformational changes of proteins by accelerating collective motions obtained from principal component analysis. ***J Chem Theory Comput*** 10, 2014
21. Wen, B.#, **Peng, J.#**, Zuo, X., Gong, Q., and Zhang, Z. Characterization of protein flexibility using small-angle x-ray scattering and amplified collective motion simulations. Biophys J 107, 2014 (**# co-first author**)

TEACHING & MENTORSHIP

Mentor for Sara Skarabot in single cell RNA-sequencing analysis — 2023
Current status: High school student intern at Stuyvesant High School

Mentor for lab members in comparative genomics and computational biophysics analysis — Since 2020
McDonald–Kreitman test, orthoMCL, dN/dS, AlphaFold, Protein structure analysis, etc.

Mentor for Chuang Yuan in molecular dynamics (MD) simulations and data analysis (master's thesis) — 2016
Current status: Research assistant at Shandong University

Mentor for Zhiyuan Ding in MD simulations of nucleosome assembly (undergraduate thesis) — 2016
Current status: PhD student at Fudan University

Mentor for lab members in biophysical data analysis — 2014-2017
Small-angle X-ray Scattering (SAXS), NMR spectroscopy data analysis, Structural modeling integrating biophysics data

Teaching assistant, Molecular Modeling of Biomacromolecules at graduate level — 2014

SERVICE & OUTREACH

Faculty Search Ambassador — 2023

Navigate candidates through campus and introduce them to faculty members and resource centers, Rockefeller University Faculty Search Seminar 2023

Science Networking Host 2022

Host of virtual networking at 2022 Annual Drosophila Meeting, session of Evolution, Immunity, and the Microbiome

Ad Hoc Reviewer Since 2018

Molecular Biology and Evolution, PLOS Genetics, Genome Biology and Evolution, Journal of Molecular Evolution, Journal of Evolutionary Biology, Biology of Reproduction, PLOS One, Archives of Biochemistry and Biophysics, International Journal of Molecular Science, BioSystems, Computational Biology and Chemistry, Journal of Molecular Structure

Organizer of the first Biological System Modeling Symposium 2015

Organizer of the first campus-wide symposium that connects scientists who study biological systems by computational modeling and simulations in USTC

Science Outreach Volunteer 2014, 2015, 2016

Introduce science and provide hands-on scientific experiments to elementary, middle, and high school students from all over the country in the Science and Technology Activity Week, School of Life Sciences, USTC

PROFESSIONAL MEMBERSHIP

Society of Molecular Biology and Evolution Since 2020

Genetic Society of America Since 2020