JUNHUI PENG, PhD

Laboratory of Evolutionary Genetics and Genomics
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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

RESEARCH EXPERIENCES

Postdoctoral Researcher, Rockefeller University Jul 2019 – present
Laboratory of Evolutionary Genetics and Genomics
Advisor: Dr. Li Zhao

- Developed a computational platform to study the origination and evolution of the interactions between sex peptide and sex peptide receptor.
- Developed a computational pipeline to identify *Drosophila* specific *de novo* genes and study their origination and protein structure evolution.
- Demonstrated how intermolecular interactions drive protein sequence adaptative evolution in *Drosophila melanogaster* by comparative genomics analysis and populational genomics analysis.
- Collaborated with colleagues in comparative genomic analysis, populational genomics analysis, and computational biophysics studies.

Postdoctoral Researcher, Hong Kong University of Science and Technology (HKUST) Oct 2017 – Jun 2019
Department of Chemistry
Advisor: Dr. Xuhui Huang

- Studied nucleosome dynamics by molecular dynamics simulations and Markov State Model.
- Collaborated with colleagues in computational biophysics and computational chemistry studies.

Postgraduate studies, USTC Sep 2012 – Jun 2017
School of Life Sciences
Advisor: Dr. Zhiyong Zhang & Dr. Yunyu Shi

- Developed a computational biophysics platform that integrates real world biophysical data to study the structure and dynamics of biomolecules.
- Collaborated with colleagues in computational biophysics studies.

Undergraduate studies, USTC Sep 2011 – Jun 2012
School of Life Sciences
Advisor: Zhiyong Zhang & Yunyu Shi

HONORS AND AWARDS

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
National Graduate Scholarship, Ministry of Education, China	2016
National Graduate Scholarship, Ministry of Education, China	2014
Outstanding Student Scholarship Bronze Award, USTC	2011
iGEM Gold Medal, International Genetically Engineered Machine Competition	2011
Outstanding Student Scholarship Silver Award, USTC	2010
Outstanding Student Scholarship Silver Award, USTC	2009

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 *(selected, more information at my google scholar profile)*

Postdoctoral research, Rockefeller University

1. **Peng, J.**, Svetec, N., Molina N., Zhao L. *The origin and evolution of the interactions between sex peptide and sex peptide receptor*. 2023 (manuscript submitted)
2. **Peng, J.**, Zhao, L. *The origin and structural evolution of de novo genes in Drosophila*. ***Biorxiv*** 2023.03.13.532420, 2023 (manuscript under revision)
3. 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***, 2023 (in press)
4. 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(6620), 2022
5. **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
6. 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

7. 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

8. 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
9. 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
10. **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

11. **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**)
12. **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**)
13. 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
14. Cheng, P.#, **Peng, J.#**, and Zhang, Z. (2017). SAXS-Oriented Ensemble Refinement of Flexible Biomolecules. Biophys J 112, **(# co-first author**)
15. 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
16. 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
17. **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
18. 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
19. **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
20. 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**)

MENTORSHIP EXPERIENCES

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

Mentor for Chuang Yuan in molecular dynamics simulations and data analysis 2016
Current status: Research assistant at Shandong University

Mentor for Zhiyuan Ding in molecular dynamics simulations of nucleosome assembly 2016
Current status: PhD student at Fudan University

Mentor for lab members in comparative genomics analysis since 2020

SERVICE & OUTREACH

Faculty Search Ambassador 2023
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
Journal of Molecular Evolution, Journal of Evolutionary Biology, Biology of Reproduction, PLOS One, International Journal of Molecular Science, Archives of Biochemistry and Biophysics, BioSystems, Computational Biology and Chemistry, Journal of Molecular Structure

PROFESSIONAL MEMBERSHIP

Society of Molecular Biology and Evolution since 2020

Genetic Society of America since 2020