

Curriculum Vitae

JUNHUI PENG

Laboratory of Evolutionary Genetics and Genomics,
The Rockefeller University, New York, NY, USA

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EDUCATION

- Ph.D.** University of Science and Technology of China July 2017
Computational Biology, School of Life Sciences
Advisor: Zhiyong Zhang & Yunyu Shi
- B.S.** University of Science and Technology of China July 2012
Biology, School of Life Sciences

RESEARCH EXPERIENCES

- Postdoctoral Researcher** Jul 2019 – present
Laboratory of Evolutionary Genetics and Genomics
The Rockefeller University
Advisor: Li Zhao
- Postdoctoral Researcher** Oct 2017 – Jun 2019
Department of Chemistry
The Hong Kong University of Science and Technology
Advisor: Xuhui Huang
- Postgraduate studies** Sep 2012 – Jun 2017
School of Life Sciences
University of Science and Technology of China
Advisor: Zhiyong Zhang & Yunyu Shi
- Undergraduate studies** Sep 2011 – Jun 2012
School of Life Sciences
University of Science and Technology of China
Advisor: Zhiyong Zhang & Yunyu Shi

HONORS AND AWARDS

- 2021:** C. H. Li Memorial Scholar Fund Award
- 2017:** CAS President Award (Excellence Award) 2017
- 2016:** National Graduate Scholarship 2016
- 2014:** National Graduate Scholarship 2014
- 2011:** Outstanding Student Scholarship Bronze Award 2011
- 2011:** iGEM Gold Medal 2011
- 2010:** Outstanding Student Scholarship Silver Award 2010
- 2009:** Outstanding Student Scholarship Silver Award 2009

SKILLS

Programming skills: C, Python, Bash

PRESENTATIONS

- 2022:** “*Intermolecular interactions drive protein adaptive and co-adaptive evolution at both species and population levels*”.
Poster presentation, the63rd Annual Drosophila Research Conference, April 6-10, 2022.

2021: “Intermolecular interactions drive protein adaptive and co-adaptive evolution at both species and population levels”. Contributed talk, the 2nd AsiaEvo Conference, August 16-19, 2021.

2014: “ACM-PCA enhanced sampling method in molecular dynamics simulation and its application in interpreting small angle X-ray scattering (SAXS) data”. Young scientists and graduate student forum, the Chinese Society of Biochemistry and Molecular Biology 2014 National Meeting, August 21-23, 2014. Xiamen, China

PUBLICATIONS (more information: [my google scholar profile](#))

• First author and co-first author

1. **Junhui Peng**, N Svetec, Li Zhao: Intermolecular interactions drive protein adaptive and co-adaptive evolution at both species and population levels. **Molecular Biology and Evolution** 2022; 39 (1).
2. **Junhui Peng**, Chuang Yuan, Xinfan Hua and Zhiyong Zhang: Molecular mechanism of histone variant H2A. B on stability and assembly of nucleosome and chromatin structures. **Epigenetics & chromatin** 2020; 13(1).
3. **Junhui Peng**, Chuang Yuan, Rongsheng Ma, Zhiyong Zhang: Backmapping from Multiresolution Coarse-Grained Models to Atomic Structures of Large Biomolecules by Restrained Molecular Dynamics Simulations using Bayesian Inference. **Journal of Chemical Theory and Computation** 2019; 15(5).
4. **Junhui Peng**, Wei Wang, Yeqing Yu, Hanlin Gu and Xuhui Huang: Clustering algorithms to Analyze Molecular Dynamics Simulation Trajectories for Complex Chemical and Biological Systems. **Chinese Journal of Chemical Physics** 2018; 31(4).
5. Peng Cheng¹, **Junhui Peng**¹, Zhiyong Zhang: SAXS-oriented Ensemble Refinement of Flexible Biomolecules. **Biophysical Journal** 2017; 112(7).
6. **Junhui Peng**, Zhiyong Zhang: Unraveling low-resolution structural data of large biomolecules by constructing atomic models with experiment-targeted parallel cascade selection simulations. **Scientific Reports** 2016; 6.
7. **Junhui Peng**, Debiao Zhao, Bin Wen, Zhiyong Zhang: Determining structural models of biomolecular complexes integrating nuclear magnetic resonance, small-angle X-ray scattering and computational simulations. **Chinese Journal of Magnetic Resonance** 2015 (32).
8. Bin Wen¹, **Junhui Peng**¹, Xiaobing Zuo, Qingguo Gong, Zhiyong Zhang: Characterization of Protein Flexibility Using Small-Angle X-Ray Scattering and Amplified Collective Motion Simulations. **Biophysical Journal** 2014; 107(4).
9. **Junhui Peng**, Zhiyong Zhang: Simulating Large-Scale Conformational Changes of Proteins by Accelerating Collective Motions Obtained from Principal Component Analysis. **Journal of Chemical Theory and Computation** 2014; 10(8).

• Collaborations

1. S Durkin, M Chakraborty, A Abrieux, K Lewald, A Gadau, N Svetec, **J Peng**, M Kopyto, C Langer, J Chiu, J Emerson, L Zhao. **Mol Biol Evol**, 2021; 38(6)
2. C Pan, C Liu, **J Peng**, P Ren, X Huang. **J Comput Chem**, 2020; 41(10).
3. J Zhang, A Li, H Zou, **J Peng**, J Guo, W Wu, H Zhang, J Zhang, X Gu, W Xu, S Xu, S Liu, A Qin, JW Lam, BZ Tang. **Mater Horizons**, 08/2019.
4. J Zhang, Q Liu, W Wu, **J Peng**, H Zhang, F. Song, B He, X Wang, H Sung, M Chen, B Li, S Liu, JW Lam, BZ Tang. **ACS nano**, 2019; 13 (3).
5. D Xu, R Ma, J Zhang, Z Liu, B Wu, **J Peng**, Y Zhai, Q Gong, Y Shi, J Wu, Q Wu, Z Zhang, K Ruan. **J Phys Chem Lett**, 2018; 9(14)
6. L Xu, L Wang **J Peng**, F Li, L Wu, B Zhang, M Lv, J Zhang, Q Gong, R Zhang, X Zuo, Z Zhang, J Wu, Y Tang, Y Shi. **Structure** 2017; 25(12).
7. C Chen, P Gu, J Wu, X Chen, S Niu, H Sun, L Wu, N Li, **J Peng**, S Shi, C Fan, M Huang, C Wong, Q Gong, C Sinha, R Zhang, L Pusztai, R Rai, S Chang, M Lei. **Nat Commun** 2017; 8.
8. M Lv, C Wang, F Li, **J Peng**, B Wen, Q Gong, Y Shi, and Y Tang. **Protein cell** 2017; 8(1).
9. S Ling, W Wang, L Yu, **J Peng**, X Cai, Y Xiong, Z Hayati, L Zhang, Z Zhang, L Song, C Tian. **Sci Rep** 2016; 6.
10. N Jia, N Liu, W Cheng, Y Jiang, H Sun, L Chen, **J Peng**, Y Zhang, Y Ding, Z Zhang, X Wang, G Cai, J Wang, M Dong, Z Zhang, H Wu, H Wang, Y Chen, C Zhou. **EMBO Rep** 2015.
11. H Hu, Y Jiang, M Zhao, K Cai, S Liu, B Wen, P Lv, Y Zhang, **J Peng**, H Zhong, H Yu, Y Ren, Z Zhang, C Tian, Q Wu, M Oliveberg, C Zhang, Y Chen, C Zhou. **Sci Rep** 2015; 5.
12. Y Zhang, B Wen, **J Peng**, X Zuo, Q Gong, Z Zhang. **Protein Cell** 2015; 6(8).
13. P Chen, Z Liu, X Wang, **J Peng**, Q Sun, J Li, M Wang, L Niu, Z Zhang, G Cai, M Teng, X Li. **PLoS ONE** 2015; 10(3).
14. Y Zou, Z Shao, **J Peng**, F Li, D Gong, C Wang, X Zuo, Z Zhang, J Wu, Y Shi, Q Gong. **FEBS Lett** 2014; 588(17).

15. D Zhao, X Wang, **J Peng**, C Wang, F Li, Q Sun, Y Zhang, J Zhang, G Cai, X Zuo, J Wu, Y Shi, Z Zhang, Q Gong. *J Struct Biol* 2014; 187(2).
16. C Wang, Y Zhu, T Caceres, L Liu, **J Peng**, J Wang, J Chen, X Chen, Z Zhang, X Zuo, Q Gong, M Teng, J Hevel, J Wu, Y Shi. *Structure* 2014; 22(5).
17. J Wang, S Qin, F Li, S Li, W Zhang, **J Peng**, Z Zhang, Q Gong, J Wu, Y Shi. *Cell Res* 2014; 24(7).
18. C Wang, Y Zhu, J Chen, X Li, **J Peng**, J Chen, Y Zou, Z Zhang, H Jin, P Yang, J Wu, L Niu, Q Gong, M Teng, Y Shi. *PLoS ONE* 2014; 9(2).
19. Z Shao, W Yan, **J Peng**, X Zuo, Y Zou, F Li, D Gong, R Ma, J Wu, Y Shi, Z Zhang, M Teng, X Li, Q Gong. *Nuc Acids Res* 2013; 42(1).
20. B Wu, F Wang, J Zhang, Z Zhang, L Qin, **J Peng**, F Li, J Liu, G Lu, Q Gong, X Yao, J Wu, Y Shi. *J Struct Biol* 2012; 180(1).