

# XIAO WANG

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## EDUCATION

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**Purdue University**, West Lafayette, U.S. Aug, 2018 – Present

*Ph.D.* in Computer Science GPA: **3.91/4.0**

Area: Computational Biology, Machine Learning, Self-Supervised Learning

**Xi'an JiaoTong University**, Xi'an, China Aug, 2014 – June, 2018

*B.S.* in Computer Science GPA: 90.57/100; Rank: **1/170**

Area: Intelligent Transportation, Machine Learning

**Graduated with highest honors, Top 10 Outstanding Student (10/4000+)**

## RESEARCH INTERESTS

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### *Computational Biology*

- 1) Macromolecular structure modeling and evaluation from experimental data (eg. Cryo-EM).
- 2) Macromolecular structure prediction and evaluation from sequence (gene) information.
- 3) Function of macromolecule prediction via sequence and structure information.

### *Machine Learning*

- 1) Development of *novel, efficient* and *general* Self-Supervised Learning (SSL) algorithms (eg. adversarial SSL, asymmetrical SSL).
- 2) Applications of self-supervised learning on biology, medicine, health.

## HONORS AND AWARDS

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**NSF MolSSI Software Fellowship** (10 across U.S, \$80,000) 2022

**Chiang Chen Overseas Fellowship** (10 across China, \$50,000) 2018

**HIWIN Outstanding Student Scholarship** (Top 0.3% , \$10,000 CNY) 2018

**Top 10 Outstanding Undergraduate of Xi'an Jiaotong University** 2017

**National Scholarship** (Top 1%, \$ 8,000 CNY) 2016

## EXPERIENCE

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**Facebook AI Research**, Menlo Park, U.S May, 2021 – Aug, 2021

*Research Scientist Intern* Advisor: Dr. Xinlei Chen, Dr. Yuandong Tian, Haoqi Fan

*Asymmetrical self-supervised learning*

**Kihara Bioinformatics Lab**, West Lafayette, U.S Aug, 2018 – Present

*Ph.D. Research Assistant* Advisor: Prof. Daisuke Kihara

*Macromolecule structure prediction, modeling and evaluation via machine learning algorithms*

**JD AI Research**, Mountain View, U.S May, 2020 – Dec, 2020

*Research Scientist Intern* Advisor: Dr. Jingen Liu, Prof. Jiebo Luo

*Temporal video event segmentation via self-supervised learning*

**Futurewei AI Lab**, Bellevue, U.S May, 2019 – August, 2019

*Research Scientist Intern* Advisor: Prof. Guojun Qi, Prof. Jiebo Luo

*Pre-task self-supervised learning and adversarial self-supervised learning.*

**Tsinghua University**, Beijing, China

June, 2016 – Jan, 2019

*Research Intern* Advisor: Prof. Li-Li, Prof. Fei-Yue Wang

*Car-following behavior prediction and traffic simulation by deep learning.*

**Institute of Automation, Chinese Academy of Sciences**, Beijing, China June, 2016 – June, 2017

*Research Intern* Advisor: Dr. Xiwei Liu, Prof. Fei-Yue Wang

*Intelligent education by deep learning.*

## SELECTED PUBLICATIONS

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### Computational Biology

#### Pre-print

- 1 **Xiao Wang**, Genki Terashi, & Daisuke Kihara. “Cryo-READ: DNA/RNA dE novo Atomic structure modeling in cryo-EM maps with deep learning”. *Science*. (2022). (Submitted).
- 2 Genki Terashi, **Xiao Wang**, Sai Raghavendra Maddhuri Venkata Subramaniya & Daisuke Kihara. “Deep-Mainmast: De novo Protein Structure Modeling for cryo-EM with Deep Learning”. *Nature Methods*. (2022). (Submitted).
- 3 Genki Terashi, **Xiao Wang** & Daisuke Kihara. “Protein Model Refinement for Cryo-EM Maps Using DAQ score”. *Acta Crystallographica Section D: Structural Biology*. (2022). (Minor Revision). [Paper] [GitHub][Colab]

#### Published

- 1 **Xiao Wang\***, Genki Terashi\*, Sai Raghavendra Maddhuri Venkata Subramaniya, John J. G. Tesmer Daisuke Kihara. “Residue-Wise Local Quality Estimation for Protein Models from Cryo-EM Maps.” *Nature Methods*. (2022). [Paper][GitHub] [Colab] [Integrated by SBGrid and Scipon for wider use in structural biology.](#)
- 2 **Xiao Wang**, Eman Alnabati, Tunde W Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi & Daisuke Kihara. “Emap2sec+: Structure Detection in Intermediate Resolution Cryo-EM Maps Using Deep Learning”. *Nature Communications*. (2021). [Paper] [GitHub][CodeOcean] [Integrated by SBGrid and Scipon for wider use in structural biology.](#)
- 3 **Xiao Wang**, Sean T, Flannery, Daisuke Kihara. “Protein Docking Model Evaluation by Graph Neural Networks”. *Frontiers in Molecular Biosciences (FMOLB)*. (2021). [Paper] [GitHub] [Recognized as representative deep-Learning-based method to directly tackle key bottleneck of structure quality assessment by CAPRI community.](#)
- 4 **Xiao Wang**, Genki Terashi, Charles W. Christoffer, Mengmeng Zhu, and Daisuke Kihara, “Protein Docking Model Evaluation by 3D Deep Convolutional Neural Networks”. *Bioinformatics* 36: 2113-2118 (2020). [Paper] [GitHub][Platform] [Recognized as representative deep-Learning-based method to directly tackle key bottleneck of structure quality assessment by CAPRI community.](#)
- 5 **Xiao Wang\***, Mizu Kittaka\*, Yilin He, Yiwei Zhang, Yasuyoshi Ueki, and Daisuke Kihara. “OC\_Finder: A deep learning-based software for osteoclast segmentation, counting, and classification”. *Frontiers in Bioinformatics*. (2021). [Paper] [GitHub] [Colab]

### Self-Supervised Learning

#### Pre-print

- 1 **Xiao Wang**, Yuhang Huang, Dan Zeng, Guo-Jun Qi. “CaCo: Both Positive and Negative Samples are Directly Learnable via Cooperative-adversarial Contrastive Learning”. *IEEE Transactions on Pattern Analysis and Machine Intelligence (IEEE T-PAMI)*. (2022). (Major Revision). [Paper] [GitHub]
- 2 **Xiao Wang**, Ying Wang, Ziwei Xuan, Guo-Jun Qi. “AdPE: Adversarial Positional Embeddings For MIM Pretraining of Transformers”. *The Eleventh International Conference on Learning Representations (ICLR 2023)*. (Submitted). [Paper] [GitHub]
- 3 **Xiao Wang**, Jingen Liu, Tao Mei, Jiebo Luo. CoSeg: “Cognitively Inspired Unsupervised Generic Event Segmentation”. *IEEE Transactions on Neural Networks and Learning Systems (IEEE TNNLS)*. (minor revision). [Paper][GitHub]

#### Published

- 1 **Xiao Wang\***, Haoqi Fan\*, Yuandong Tian, Daisuke Kihara, Xinlei Chen. “On the Importance of Asymmetry for Siamese Representation Learning”. *IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR 2022)*. [Paper] [GitHub] [First asymmetrical self-supervised learning approach](#).
- 2 **Xiao Wang**, Guo-Jun Qi. “Contrastive Learning with Stronger Augmentations”. *IEEE Transactions on Pattern Analysis and Machine Intelligence (IEEE T-PAMI)*. (2022). [Paper] [GitHub]
- 3 **Xiao Wang\***, Qianjiang Hu\*, Wei Hu, Guo-Jun Qi. AdCo: “Adversarial Contrast for Efficient Learning of Unsupervised Representations from Self-Trained Negative Adversaries”. *IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR 2021)*. [Paper] [GitHub]. [Pioneering work in adversarial self-supervised learning](#).
- 4 Guo-Jun Qi, Liheng Zhang, Feng Lin, **Xiao Wang**. “Learning Generalized Transformation Equivariant Representations via Autoencoding Transformations”. *IEEE Transactions on Pattern Analysis and Machine Intelligence (IEEE T-PAMI)*. (2020). [Paper] [GitHub]
- 5 **Xiao Wang**, Daisuke Kihara, Jiebo Luo, Guo-Jun Qi. “Enaet: Self-trained ensemble autoencoding transformations for semi-supervised learning”. *IEEE Transactions on Image Processing (IEEE TIP)*. (2020). [Paper] [GitHub] [Pioneering work in integrating self-supervised learning for semi-supervised learning](#).

### Intelligent Transportation (before Ph.D.)

- 1 **Xiao Wang**, Rui Jiang, Li Li, Yi-Lun Lin, and Fei-Yue Wang. “Long memory is important: A test study on deep-learning based car-following model”. *Physica A: Statistical Mechanics and its Applications*, 514: 786-795, (2019) [Paper]
- 2 **Xiao Wang**, Rui Jiang, Li Li, Yilun Lin, Xinhua Zheng, and Fei-Yue Wang. “Capturing car-following behaviors by deep learning”. *IEEE Transactions on Intelligent Transportation Systems (IEEE T-ITS)*, PP(99):1–11, (2018). [Paper] [Nominated for George N. Saridis Best Transactions Paper Award](#).

\* denotes equal contribution.

### PRESENTATIONS & TALKS

- 1 Invited Talk: “Macromolecular Structure Modeling and Evaluation by Deep Learning”, **Xiao Wang**, King Abdullah University of Science and Technology (KAUST), Oct 24th, 2022.
- 2 Invited Talk: “Macromolecular Structure Modeling and Evaluation by Deep Learning”, **Xiao Wang**, The University of Hong Kong (HKU), Oct 17th, 2022.
- 3 Invited Talk: “The GRU-based Car-Following Model.”, **Xiao Wang**, Rui Jiang, Li Li, Yilun Lin, Xinhua Zheng, and Fei-Yue Wang. Institute of Automation, Chinese Academy of Sciences, Aug 15, 2022.
- 4 Invited Talk: “How to achieve adversarially self-supervised learning?”, **Xiao Wang**, Qianjiang Hu, Yuhang Huang, Wei Hu, Zeng Dan, Guo-Jun Qi. TechBeat, Aug 4, 2022.
- 5 Invited Talk: “De novo DNA/RNA structure modeling from cryo-EM maps by deep learning.”, **Xiao Wang**, Genki Terashi, Daisuke Kihara. The Molecular Sciences Software Institute, Virginia Tech, June 29, 2022.
- 6 Presentation: “On the Importance of Asymmetry for Siamese Representation Learning.”, **Xiao Wang\***, Haoqi Fan\*, Yuandong Tian, Daisuke Kihara, Xinlei Chen. CVPR 2022 Representation Learning Session. June 22, 2022.
- 7 Invited Talk: “Adversarial self-supervised learning”, **Xiao Wang**, Qianjiang Hu, Wei Hu, Guo-Jun Qi. Huawei Central Research. May 16th, 2022.
- 8 Invited Talk: “Pre-task and contrastive self-supervised learning”, **Xiao Wang**, OPPO AI Research, March 11th, 2022.
- 9 Presentation: “Deep learning-based local quality estimation for protein structure models from cryo-EM maps”, Genki Terashi\*, **Xiao Wang\***, Sai Raghavendra Maddhuri Venkata Subramaniya, John J. G. Tesmer, Daisuke Kihara, 66th Biophysical Society Annual Meeting, San Francisco, Feb. 19-23, 2022
- 10 Invited Talk: “Pre-task and contrastive self-supervised learning”. **Xiao Wang**, Meta AI, Feb 22th, 2022.
- 11 Invited Talk: “Pre-task and contrastive self-supervised learning”. **Xiao Wang**, Microsoft Research, Dec 10th, 2021.
- 12 Invited Talk: “Introduction of self-supervised learning”. **Xiao Wang**, Google Brain, Nov 29th, 2021.
- 13 Invited Talk: “Pre-task and contrastive self-supervised learning”. **Xiao Wang**, VISA AI Research, Nov 12th, 2021.
- 14 Presentation: “The OC\_Finder: A deep learning-based software for in vitro osteoclast counting”, **Xiao Wang**, Mizuho Kittaka, Yilin He, Yiwei Zhang, Daisuke Kihara, Yasuyoshi Ueki, 2021 Annual Meeting of

The American Society for Bone and Mineral Research, October 1-4, 2021.

- 15 Presentation: "Emap2sec+: Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning.", **Xiao Wang**, Eman Alnabati, Tunde W. Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, 71st Annual Meeting of the American Crystallographic Association, July 30 - Aug 5, 2021.
- 16 Presentation: "Asymmetrical self-supervised learning. ", **Xiao Wang\***, Haoqi Fan\*, Yuandong Tian, Daisuke Kihara, Xinlei Chen. Facebook AI CV group, July 24, 2021.
- 17 Presentation: "Adversarial Contrast for Efficient Learning of Unsupervised Representations from Self-Trained Negative Adversaries", **Xiao Wang**, Qianjiang Hu, Wei Hu, Guo-Jun Qi. CVPR 2021 Representation Learning Session. June 17, 2022.
- 18 Invited Talk: "Adversarial self-supervised learning", **Xiao Wang**, Qianjiang Hu, Wei Hu, Guo-Jun Qi, Microsoft Research Asia, May 15, 2021.
- 19 Presentation: "Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning", **Xiao Wang**, Eman Alnabati, Tunde W. Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, The Hitchhiker's Guide to the Biomolecular Galaxy 2021, May 12-13, 2021.
- 20 Presentation: "Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning", **Xiao Wang**, Eman Alnabati, Tunde W. Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, 2021 65th Biophysical Society Annual Meeting, February 22-26, 2021.
- 21 Presentation: "Emap2sec+: Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning", **Xiao Wang**, Eman Alnabati, Tunde Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, Frontiers in Cryo-Electron Microscopy, Keystone Symposia, Feb. 3-4, 2021.
- 22 Invited Talk: "Adversarial self-supervised learning.", **Xiao Wang**, Qianjiang Hu, Wei Hu, Guo-Jun Qi. Facebook AI Research, Jan 20, 2021.
- 23 Presentation: "Protein Docking Model Evaluation by Graph Neural Networks", **Xiao Wang**, Sean T. Flannery, Daisuke Kihara, Structural and Computational Biology and Biophysics (SCBB) Graduate Student Symposium of Purdue, Dec 16, 2020.
- 24 Presentation: "Emap2sec+: Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning", **Xiao Wang**, Eman Alnabati, Tunde Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, 5th Annual Southern California Cryo-EM Symposium, Oct 30, 2020.
- 25 Guest Lecture: "Review of car-following model", **Xiao Wang**, Institute of Automation, Tsinghua University, April 21, 2020.
- 26 Presentation: "Protein docking model evaluation by 3D convolutional neural networks", **Xiao Wang**, Genki Terashi, Charles W Christoffer, Mengmeng Zhu, Daisuke Kihara, invited talk by Aggregate Intellect - AI.SCIENCE, Mar 24, 2020. [Video].

## PROFESSIONAL SERVICES

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*Reviewer of IEEE Transactions on Pattern Analysis and Machine Intelligence (IEEE-T-PAMI)*

*Reviewer of IEEE Transactions on Image Processing (IEEE-TIP)*

*Reviewer of Pattern Recognition*

*Reviewer of Bioinformatics*

*Reviewer of IEEE Transactions on Intelligent Transportation Systems (IEEE-T-ITS)*

*Reviewer of IEEE Transactions on Multimedia (IEEE-TMM)*

*Reviewer of ACM Transactions on Knowledge Discovery from Data (IEEE-TKDD)*

*Reviewer of IEEE Intelligent Systems*

*Reviewer of Frontiers in Bioinformatics*

*Reviewer of Conference on Neural Information Processing Systems (NeurIPS)*

*Reviewer of Conference on Computer Vision and Pattern Recognition (CVPR)*

*Reviewer of International Conference on Computer Vision (ICCV)*

*Reviewer of European Conference on Computer Vision (ECCV)*

## TEACHING & MENTORING EXPERIENCE

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### Teaching

*Computing for Life Sciences, Purdue*

Fall 2020

*Java Programming, XJTU*

Spring 2017

### Guest Lecture

*Traffic Flow Theory, Tsinghua*

April, 2020

*Molecular Sciences, Virginia Tech*

July, 2020

### Mentoring

Grace Su, undergraduate from Columbia University

2021-2022

Yunhan Huang, undergraduate student from Purdue University

2021-2022

Yuhang Huang, undergraduate from Shanghai University

2021-2022

Rohan Raghavan Narasimha, M.S. graduate student from Purdue University

2020-2021

Sean T Flannery, M.S. graduate student from Purdue University

2020-2021

Qianjiang Hu, undergraduate from Peking University

2020-2021

Yilin He, undergraduate summer intern from Shandong University

2019

Yiwei Zhang, undergraduate summer intern from Rensselaer Polytechnic Institute

2019

## OPEN SOURCE PROJECT

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### DAQ-Refine

DAQ-Refine is a protein structure refinement tool by DAQ-score and ColabFold.

Available at: <https://github.com/kiharalab/DAQ-Refine> and <https://bit.ly/DAQ-Refine>.

### Asym-Siam

Asym-Siam experimentally verified the importance of asymmetry for Siamese Representation Learning with obvious improvement.

Available at: <https://github.com/facebookresearch/asym-siam>.

### DAQ

DAQ is a software accesses the quality of protein models built from cryo-Electron Microscopy (EM) maps, which uses local map density features captured by deep learning.

Available at: <https://github.com/kiharalab/DAQ> and <https://bit.ly/daq-score>.

## CaCo

CaCo is a state-of-the-art cooperative-adversarial contrastive learning method where both positive and negative samples are directly learnable.

Available at: <https://github.com/maple-research-lab/caco>.

## CaSeg

CoSeg is a self-supervised learning-based event boundary detection method.

Available at: <https://github.com/wang3702/CoSeg>.

## OC\_Finder

OC\_Finder is a computational tool using deep learning for fully automated osteoclast segmentation, classification, and counting.

Available at: [https://github.com/kiharalab/OC\\_Finder](https://github.com/kiharalab/OC_Finder).

## CLSA

CLSA is a general contrastive learning framework by introducing the information from stronger augmentation.

Available at: <https://github.com/maple-research-research-lab/CLSA>.

## GNN\_DOVE

GNN\_DOVE is a software can evaluate the quality of protein-docking models using graph neural networks by reformulating protein structures as graphs.

Available at: [https://github.com/kiharalab/GNN\\_DOVE](https://github.com/kiharalab/GNN_DOVE).

## GNN\_Pocket

GNN\_Pocket is a software that can detect protein pockets with graph neural network.

Available at: [https://github.com/kiharalab/GNN\\_Pocket](https://github.com/kiharalab/GNN_Pocket).

## AdCo

AdCo is an algorithm for effective self-supervised learning through adversarial training of negative examples.

Available at: <https://github.com/maple-research-lab/AdCo>.

## Emap2sec+

Emap2sec+ is a software detects local structure information of proteins and DNA/RNA in cryo-EM maps using deep learning.

Available at: <https://github.com/kiharalab/Emap2secPlus> and <https://doi.org/10.24433/C0.7165707.v1>.

## Attention\_AD

Attention\_AD is a software that can distinguish active and inactive peptides for gene expression using Long Short Term Memory (LSTM).

Available at: [https://github.com/kiharalab/Attention\\_AD](https://github.com/kiharalab/Attention_AD).

## EnAET

EnAET is a software that benefits semi-supervised learning via self-trained ensemble auto-encoding transformations.

Available at: <https://github.com/maple-research-lab/EnAET>.

## DOVE

DOVE is a software can evaluate the quality of protein-docking models using 3D neural networks.

Available at: <https://github.com/kiharalab/DOVE> and <https://kiharalab.org/dove>.

## SKILLS

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- Expertise: Pytorch, Python, Tensorflow, Matlab, Java
- Capable: SQL, C, C++, Fortran, Java Web, Latex, Android