Yuanqing Wang

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Academic Positions

2021-Current Adjunct Assistant Professor
City College of New York
New York, N.Y.

Education

2018-Current **Ph.D.** Candidate
Physiology, Biophysics, and System Biology
Research interest: Graph learning for molecule and protein topology
P.I.: Prof. John D. Chodera
Memorial Sloan Kettering Cancer Center and
Weill Cornell Medical College
New York, N.Y.

2019-Current **M.F.A.** Student
Creative Writing—short fiction
City College of New York
Harlem, New York, N.Y.

2019-2021 **Master of Bussiness Administration** (Online)
Quantic School of Business and Technology
Washington, D.C.

2016-2018 **Bachelor of Science** with *Honor*
Major: Comparative Literature and Chemistry
Theses: *Folklore Music Renaissance in Comtemporary China* (with Prof. Xiaobing Tang) and *In Silico Discovery of Iron Chelators* (with Prof. Nouri Neamati)
University of Michigan
Ann Arbor, Mich.

2014-2016 **Bachelor of Science** – Ministry of Education Plan Everest
Major: Chemistry
Undergraduate Research: *Transition Metal-Catalyzed Synthesis Methodology* and *Design of Dye-Sensitized Solar Cells.* (with Prof.Jingsong You)
Sichuan University
Chengdu, P.R.China

Publications

Wang Y and Karaletsos T. Stochastic Aggregation in Graph Neural Networks. [arXiv:2102.12648]

Wang Y, Fass J, and Chodera JD. End-to-End Differentiable Molecular Mechanics Force Field Construction. [arXiv:2010.01196]

Wang Y, Nguyen M, Retchin M, Karaletsos T, and Chodera JD. Bayesian Active Drug Discovery. [https://realworldml.github.io/files/cr/48_BADD_paper_workshop.pdf] (ICML RealML Workshop)

Wang Y, Fass J, Stern C, Luo K, and Chodera JD. Graph nets for partial charge prediction. [arXiv:1909.07903] (NIPS Physics ML workshop)

Wade AD, Rizzi A, **Wang Y**, and Huggins DJ. Computational Fluorine Scanning Using Free-Energy Perturbation. *J. Chem. Inf. Model. 20195962776-2784.*[doi://10.1021/acs.jcim.9b00228]

Wang Y "A tale of clear broth noodles." *A Bite of the Old Times* , Chongqing Publishing House, 2016. [ISBN:9787229105013]

Presentations and Invited Talks

Oct 2019	Hypergraph Functional Potential and GN-based Partial Charge Predictions **Open Force Field Consortium Webinar** https://youtu.be/ndIgAV2Xwfk San Diego, Calif.
Oct 2019	Using Graph Nets (GNs) to predict molecular properties **PyData 2019** https://youtu.be/Al8_pbgrnTM New York, N.Y.
Aug-Sep 2019	Graph Nets for Learning Molecular Physics **BenevolentAI** Guest Talk London, U.K. **2nd Royal Society of Chemistry A.I. in Chemistry** Cambridge, U.K. **Weill Cornell Biophysics Symposium** New York, N.Y.

Scholarships, Fellowships, Honors and Awards

2021 **Anagenex, Inc.**
Distinguished Open Science Fellowship

2021 **The Irwin and Alice Stark Short Fiction Awards**

2018-2019 **Cornell University Weill Cornell Medical College**
Full Scholarship $ 76,950 each year

2017 **University of Michigan UROP**
Biomedical and Life Sciences Summer Fellowship

Oct 2014 -Jun 2016 **Ministry of Education** and **Ministry of Finance** of P.R. China
Pilot Plan for Forstering Top-notch Students in Basic Science

Jan 2015 Jun 2015 National Scholarship for Students in
Jan 2016 Jun 2016 Pilot Plan for Forstering Top-notch Students in Basic Science
(Consecutively Four Times) *First Class*

2013 **Yangtse Evening Post**
Distinguished Student Writer

Industry Positions

2021 Machine Learning Software Engineering Ph.D. Intern
Facebook Dating, **Facebook, Inc.**
New York, N.Y. and Menlo Park, Calif.

2019-2020 Co-founder, Vice President
Uli (Shenzhen) Technology Co. Ltd.
Shenzhen, P.R. China

2019-2020 Co-founder, Vice President
Uli, Inc.
New York, N.Y.

Volunteer Experiences

2017-2018 Speakers Coach
TEDxUofM
Ann Arbor, Mich.

2016 Instructor
Chengdu Autism Center
Chengdu, P.R. China

2016 Subtitle Translator
coursera.org

2016 English Instructor
Siem Reap, Cambodia

Open Source Software Developments

pinot[https://github.com/choderalab/pinot]: Probabilistic Inference for Novel Therapeutics Design
espaloma[https://github.com/choderalab/espaloma]: Extensible Surrogate Potential of Ab initio Learned and Optimized by Message-passing Algorithms