

# Yuanqing Wang

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## EDUCATION

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- 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  
**the City College of the City University 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

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- Wang Y** and Karaletsos T. Stochastic Aggregation in Graph Neural Networks. [[arXiv:2102.12648](https://arxiv.org/abs/2102.12648)]
- Wang Y**, Fass J, and Chodera JD. End-to-End Differentiable Molecular Mechanics Force Field Construction. [[arXiv:2010.01196](https://arxiv.org/abs/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](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](https://arxiv.org/abs/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

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- 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](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

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- 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

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- 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

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- 2017-2018    Speakers Coach  
**TEDxUofM**  
Ann Arbor, Mich.
- 2016    Instructor  
**Chengdu Autism Center**  
Chengdu, P.R. China
- 2016    Subtitle Translator  
[coursera.org](https://www.coursera.org)
- 2016    English Instructor  
Siem Reap, Cambodia

## OPEN SOURCE SOFTWARE DEVELOPMENTS

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**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