

JUNTENG JIA

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🎓 EDUCATION

- **Ph.D. in Computer Science** Field: Scientific Computing
Cornell University May 2021
- **M.S. in Computer Science** GPA: 4.10/4.30
Cornell University May 2020
- **M.S. in Chemistry** GPA: 4.00/4.30
Cornell University August 2017
- **B.S. in Chemistry** GPA: 3.78/4.00
Nanjing University September 2015

👤 PROFESSIONAL EXPERIENCE

- **Research Scientist** Artificial Intelligence
Facebook June 2021 –
- **Software Engineer Intern** Messenger Business Ranking
Facebook Summer 2020
- **Software Engineer Intern** Data Infrastructure & Analysis
Google Summer 2019

🏆 AWARDS & HONORS

- Global Top 100 Chinese Rising Stars in Artificial Intelligence, Baidu 2021
- KDD Travel Award, Association for Computing Machinery 2019
- Exchange Student Scholarship, University of Sydney 2014
- China National Scholarship (Top 0.1%) 2013
- Renmin Scholarship, Nanjing University 2012

📖 PUBLICATIONS

(* means co-first authors)

1. Graph Belief Propagation Networks.
Junteng Jia, Cenk Baykal, Vamsi K. Potluru, and Austin R. Benson.
(Under Review for) *Proceedings of the International Conference on Knowledge Discovery & Data Mining*, 2022
2. A Unifying Generative Model for Graph Learning Algorithms.
Junteng Jia, and Austin R. Benson.
SIAM Journal on Mathematics of Data Science, 2022
3. Residual Correlation in Graph Neural Network Regression.
Junteng Jia, and Austin R. Benson.
Proceedings of the International Conference on Knowledge Discovery & Data Mining, 2020.
4. Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics.
Hsin-Yu Ko, **Junteng Jia**, Biswajit Santra, Xifan Wu, Roberto Car, and Robert A. DiStasio Jr.
Journal of Chemical Theory and Computation, 2020
5. Neural Jump Stochastic Differential Equations.
Junteng Jia, and Austin R. Benson.
Advances in Neural Information Processing Systems, 2019.
6. Graph-based Semi-Supervised & Active Learning for Edge Flows.
Junteng Jia, Michael T. Schaub, Santiago Segarra, and Austin R. Benson.
Proceedings of the International Conference on Knowledge Discovery & Data Mining, 2019.

7. Random Spatial Network Models for Core-Periphery Structure.
Junteng Jia, and Austin R. Benson.
Proceedings of the International Conference on Web Search and Data Mining, 2019.
8. On the Geometric Dependence of the Molecular Dipole Polarizability in Water.
Ka Un Lao, **Junteng Jia**, Rahul Maitra, and Robert A. DiStasio Jr.
The Journal of Chemical Physics, 2019
9. Unraveling Substituent Effects on the Glass Transition Temperatures of Biorenewable Polyesters.
Xiaopeng Yu*, **Junteng Jia***, Shu Xu, Ka Un Lao, Maria J. Sanford, Ramesh K. Ramakrishnan, Sergei I. Nazarenko, Thomas R. Hoye, Geoffrey W. Coates, and Robert A. DiStasio Jr.
Natural Communication, 2018
10. Exploiting Molecular Weight Distribution Shape to Tune Domain Spacing in Block Copolymer Thin Films.
Dillon T. Gentekos*, **Junteng Jia***, Erika S. Tirado, Katherine P. Barteau, Detlef-M. Smilgies, Robert A. DiStasio Jr., and Brett P. Fors.
Journal of the American Chemical Society, 2018
11. Advanced Capabilities for Materials Modelling with Quantum ESPRESSO.
Paolo Giannozzi, Oliviero Andreussi, Thomas Brumme, Oana Bunau, Marco Buongiorno Nardelli, Matteo Calandra, Roberto Car, Carlo Cavazzoni, Davide Ceresoli, Matteo Cococcioni, Nicola Colonna, Ivan Carnimeo, Andrea Dal Corso, Stefano de Gironcoli, Pietro Delugas, Robert A. DiStasio Jr., Andrea Ferretti, Andrea Floris, Guido Fratesi, Giorgia Fugallo, Ralph Gebauer, Uwe Gerstmann, Feliciano Giustino, Tommaso Gorni, **Junteng Jia**, Mitsuaki Kawamura, Hsin-Yu Ko, Anton Kokalj, Emine Küçükbenli, Michele Lazzeri, Margherita Marsili, Nicola Marzari, Francesco Mauri, Ngoc Linh Nguyen, Huy-Viet Nguyen, Alberto Otero-de-la-Roza, Lorenzo Paulatto, Samuel Poncé, Dario Rocca, Riccardo Sabatini, Biswajit Santra, Martin Schlipf, Ari Paavo Seitsonen, Alexander Smogunov, Iurii Timrov, Timo Thonhauser, Paolo Umari, Nathalie Vast, Xifan Wu, and Stefano Baroni
Journal of Physics: Condensed Matter, 2017
12. Different Ways of Hydrogen Bonding in Water.
Yunwen Tao, Wenli Zou, **Junteng Jia**, Wei Li, and Dieter Cremer.
Journal of Chemical Theory and Computation, 2017
13. Normal Auger Processes with Ultrashort X-ray Pulses in Neon.
Raymond Sullivan, **Junteng Jia**, Álvaro Vázquez-Mayagoitia, and Antonio Picón.
Physical Review A, 2016
14. Vibrational Spectra of Molecular Crystals with the Generalized Energy-Based Fragmentation Approach.
Tao Fang, **Junteng Jia**, and Shuhua Li.
The Journal of Physical Chemistry A, 2016

TALKS

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|---|-----------------------------------|
| 1. Label Prediction on Graphs with Topological Correlations and Constraints.
JP Morgan AI Research | September 17, 2020
Virtual |
| 2. Residual Correlation in Graph Neural Network Regression.
KDD, Oral Presentation | August 27, 2020
Virtual |
| 3. Graph-based Semi-Supervised & Active Learning for Edge Flows.
KDD, Oral Presentation | August 7, 2019
Anchorage, AK |
| 4. Semi-Supervised Learning for Edge Flows.
Cornell University | February 11, 2019
Ithaca, NY |
| 5. Enabling Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics.
APS March Meeting | March 13, 2017
New Orleans, LA |

ACADEMIC SERVICES

- **Reviewer:** *NeurIPS (2020, 2021), Applied Network Science, Transactions on Information Systems, and Patterns*

TECH SKILLS

- **Languages:** Python, Julia, Java, C/C++, MATLAB
- Frameworks:** PyTorch, TensorFlow, Flux, MPI, OpenMP