Junteng Jia

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Education

- **Ph.D. in Computer Science** — Field: Graph Mining
  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** — Applied Machine Learning
  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*
- ***Renming Scholarship, Nanjing University*** *2012*

Preprints

1. A Unifying Generative Model for Graph Learning Algorithms.
   ***Junteng Jia**, and Austin R. Benson.*
   arXiv:2101.07730, 2021

Publications

(∗ means co-first authors)

1. Residual Correlation in Graph Neural Network Regression.
   ***Junteng Jia**, and Austin R. Benson.*
   Proceedings of the International Conference on Knowledge Discovery & Data Mining (KDD), 2020.
2. 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
3. Neural Jump Stochastic Differential Equations.
   ***Junteng Jia**, and Austin R. Benson.*
   Advances in Neural Information Processing Systems (NeurIPS), 2019.
4. 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 (KDD), 2019.
5. 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 (WSDM), 2019.

6. 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

7. 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

8. 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

9. 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

10. 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

11. Normal Auger Processes with Ultrashort X-ray Pulses in Neon.
    *Raymond Sullivan, **Junteng Jia**, Álvaro Vázquez-Mayagoitia, and Antonio Picón.*
    Physical Review A, 2016

12. 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

1. Label Prediction on Graphs with Topological Correlations and Constraints. — *September 17, 2020*
   JP Morgan AI Research — *Virtual*

2. Residual Correlation in Graph Neural Network Regression. — *August 27, 2020*
   KDD, Oral Presentation — *Virtual*

3. Graph-based Semi-Supervised & Active Learning for Edge Flows. — *August 7, 2019*
   KDD, Oral Presentation — *Anchorage, AK*

4. Semi-Supervised Learning for Edge Flows. — *February 11, 2019*
   Cornell University — *Ithaca, NY*

5. Enabling Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics. — *March 13, 2017*
   APS March Meeting — *New Orleans, LA*

Service

- Reviewer for *NeurIPS 2020 & 2021*, *Applied Network Science*, *Transactions on Information Systems*, *Patterns*

Tech Skills

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