Tian Xie

Curriculum Vitae

Massachusetts Institute of Technology
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Research Interests

Novel machine learning algorithms for accelerated material screening and fundamental understanding. Large scale computational systems for materials. Accelerated discovery of materials for energy innovations.

Education

2015–present **Ph.D. materials science and engineering**, *Massachusetts Institute of Technology*, Cambridge, MA, USA.
Thesis: Machine learning accelerated discovery of materials for energy applications.
Advisor: Jeffrey C. Grossman

2011–2015 **B.S. chemistry**, *Peking University*, Beijing, China.

Selected Publications

Y. Wang*, **T. Xie***, A. France-Lanord, A. Berkley, J. Johnson, Y. Shao-Horn, J. Grossman, "Towards Designing Highly Conductive Polymer Electrolyte by Machine Learning Assisted Coarse-Grained Molecular Dynamics", *Submitted*. (* equal contributions)

T. Xie, A. France-Lanord, Y. Wang, Y. Shao-Horn, J. Grossman, "Graph dynamical networks for unsupervised learning of atomic scale dynamics in materials", *Nat. Commun.* 10.1 (2019): 2667.

T. Xie, J. Grossman, "Hierarchical Visualization of Materials Space with Graph Convolutional Neural Networks", *J. Chem. Phys.*, 149.17 (2018): 174111.

Z. Ahmad, **T. Xie**, C. Maheshwari, J. Grossman, V. Viswanathan, "Machine Learning Enabled Computational Screening of Inorganic Solid Electrolytes for Dendrite Suppression with Li Metal Anode", *ACS Cent. Sci.*, 4.8 (2018): 996.

T. Xie, J. Grossman, "Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties", *Phys. Rev. Lett.* 120.14 (2018): 145301.

Research Experience

Massachusetts Institute of Technology

Research Assistant **Large scale screening of polymer electrolytes for lithium-ion battery.** (2019.09–present)
Led an effort involving 7 postdocs/students from 4 different groups to screen 10,000 polymer electrolytes for improved lithium-ion conductivity.

Automated system for designing polymer electrolytes. (2018.03–2019.05)
Developed a Bayesian optimization workflow to automatically screen the polymer electrolyte material space by running coarse-grained molecular dynamics simulation in parallel at a large scale. Determined key contributing factors for improving Li-ion conductivity in polymer electrolytes.

Unsupervised learning of atomic dynamics in materials. (2018.06–2019.02)
Designed an unsupervised learning algorithm to learn the dynamics of atoms or small molecules from molecular dynamics trajectories. Applied the algorithm to understand dynamics in amorphous material systems, including solid-liquid interfaces and solid polymer electrolytes for Li-ion batteries.

Hierarchical visualization of materials space. (2018.03–2018.06)
Explored the physical meaning of graph convolutional neural networks by developing a visualization approach. Discovered patterns that reflect material similarities at different scales in three representative classes of materials: perovskites, elemental boron, and general inorganic crystals, covering material spaces of different compositions, structures, and both, respectively.

Accelerated screening of electrolytes for lithium metal batteries. (2017.11–2018.03)
Applied graph convolutional neural network (CGCNN) to screening over 12,000 Li containing inorganic compounds and predicted their abilities to suppress dendrite formation. Used an ensemble approach to estimate prediction uncertainties during the extrapolation.

Graph convolutional neural networks for material representations. (2016.09–2017.11)
Designed the first graph convolutional neural networks framework (CGCNN) to represent arbitrary material structures. Achieved DFT accuracy for 8 different material properties and discovered of empirical rules for designing new perovskite materials.

DeepMind

Research Intern

Graph networks for materials discovery. (2019.05–2019.08)
Led an undisclosed research project that applies graph networks to materials discovery. A manuscript in process.
Host: James Kirkpatrick, Pushmeet Kohli

X (formerly Google X)

PhD Software Intern

Entrepreneurial project combining machine learning and physics. (2019.02–2019.05)
Led research efforts of a new direction for an undisclosed early stage entrepreneurial project that combines machine learning and physics. Filed a patent for a potential product as a result of the research.
Host: Brian Adolf, Martin Schubert

Stanford University

Visiting Student

Carbon nanotube based solar cells. (2014.06–2014.08)
Optimized the architecture and fabrication methods for solar cells based on carbon nanotubes.
Advisor: Zhenan Bao

Peking University

Research Assistant

Patterning two dimensional materials for optoelectronics. (2013.06–2015.07)
Developed a patterning approach for two dimensional chalcogenide crystals at a large area. Fabricated photodetector devices using the patterning approach.
Advisor: Hailin Peng, Zhongfan Liu

Publications

Massachusetts Institute of Technology

10. A. France-Lanord, Y. Wang, **T. Xie**, Y. Shao-Horn, J. Grossman, "The effect of selected variations in the chemical structure of poly(ethylene oxide)-based polymers on lithium transport in concentrated electrolytes", *Submitted*.
9. Y. Wang*, **T. Xie***, A. France-Lanord, A. Berkley, J. Johnson, Y. Shao-Horn, J. Grossman, "Towards Designing Highly Conductive Polymer Electrolyte by Machine Learning Assisted Coarse-Grained Molecular Dynamics", *Submitted*. (* equal contributions)
8. S. Gong, **T. Xie**, T. Zhu, S. Wang, E. Fadel, Y. Li, J. Grossman, "Predicting charge density distribution of materials using a local-environment-based graph convolutional network", *Phys. Rev. B*, in press.
7. **T. Xie**, A. France-Lanord, Y. Wang, Y. Shao-Horn, J. Grossman, "Graph dynamical networks for unsupervised learning of atomic scale dynamics in materials", *Nat. Commun.* 10.1 (2019): 2667.
6. **T. Xie**, J. Grossman, "Hierarchical Visualization of Materials Space with Graph Convolutional Neural Networks", *J. Chem. Phys.*, 149.17 (2018): 174111.
5. Z. Ahmad, **T. Xie**, C. Maheshwari, J. Grossman, V. Viswanathan, "Machine Learning Enabled Computational Screening of Inorganic Solid Electrolytes for Dendrite Suppression with Li Metal Anode", *ACS Cent. Sci.*, 4.8 (2018): 996.
4. **T. Xie**, J. Grossman, "Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties", *Phys. Rev. Lett.* 120.14 (2018): 145301.

Stanford University

3. G. Koleilat, M. Vosgueritchian, T. Lei, Y. Zhou, D. Lin, F. Lissel, P. Lin, John. To, **T. Xie**, K. England, Y. Zhang, Z. Bao, "Surpassing the exciton diffusion limit in single-walled carbon nanotube sensitized solar cells", *ACS Nano* 10.12 (2016): 11258.

Peking University

2. M. Wang, J. Wu, L. Lin, Y. Liu, B. Deng, Y. Guo, Y. Lin, **T. Xie**, W. Dang, Y. Zhou, H. Peng, "Chemically engineered substrates for patternable growth of two-dimensional chalcogenide crystals", *ACS nano* 10.11 (2016): 10317.
1. W. Zheng*, **T. Xie***, Y. Zhou*, Y. Chen, W. Jiang, S. Zhao, J. Wu, Y. Jing, Y. Wu, G. Chen, Y. Guo, J. Yin, S. Huang, H. Xu, Z. Liu, H. Peng, "Patterning two-dimensional chalcogenide crystals of Bi2Se3 and In2Se3 and efficient photodetectors", *Nat. Commun.* 6.1 (2015): 6972. (* equal contributions)

Talks

5. [Invited] **T. Xie**, "Graph neural networks as a general framework for the design and understanding of materials", *Computational Chemistry and Machine Learning Workshop*, Xiamen, China (2019)
4. [Invited] **T. Xie**, A. France-Lanord, Y. Wang, Y. Shao-Horn, J. Grossman, "Graph neural networks as a general framework for the design and understanding of materials", *Toyota Research Institute*, Mountain View, CA (2019)

3. **T. Xie**, J. Grossman, "CGCNN—A Graph Representation of Materials for Property Prediction and Materials Design", *MRS Fall Meeting*, Boston, MA (2018)
2. **T. Xie**, A. France-Lanord, Y. Wang, J. Grossman, "Continuous Representation of Chemical Environments for the Prediction of Material Properties", *APS March Meeting*, Los Angeles, CA (2018)
1. **T. Xie**, J. Grossman, "Graph Representation of Periodic Systems for Accurate and Explainable Prediction of Material Properties via Machine Learning", *MRS Fall Meeting*, Boston, MA (2017)

Posters

3. [Highlighted] **T. Xie**, J. Grossman, "CGCNN: a graph representation of materials for property prediction and materials design", *MRL Materials Day*, Cambridge, MA (2018)
2. **T. Xie**, A. France-Lanord, Y. Wang, Y. Shao-Horn, J. Grossman, "Understanding Lithium-ion Transport with Deep Neural Networks", *TRI Accelerated Materials Design and Discovery workshop*, Redwood City, CA (2018)
1. **T. Xie**, A. France-Lanord, Y. Wang, Y. Liu, J. Grossman, "Artificial Intelligence for Accelerated Materials Design", *MIT Intelligence Quest Launch*, Cambridge, MA (2018)

Teaching and Mentorship

2018–present **Student Mentor.** Advised multiple graduate students, undergraduates, and high school students.

1. Sheng Gong, graduate student at MIT (Jan. 2018–present).
2. William Xu, high school student visiting MIT (Jun. 2018–Aug. 2018).
3. Pierre-Paul De Breuck, graduate student visiting MIT (June. 2018–Aug. 2018).
4. Yu Tao, undergraduate student visiting MIT (Feb. 2019–present).

Fall 2016 **Teaching assistant.** Taught *6.009 Fundamentals of Programming* at MIT, helped over 200 students with 10 different Python projects, and designed 2 sets of quiz questions.

Service

Open Source **Open source project leader.** Wrote 2 popular open source software packages for machine learning accelerated discovery of materials.

- Crystal Graph Convolutional Neural Networks (CGCNN): `https://github.com/txie-93/cgcnn`. (Over 100 stars at GitHub, incorporated in 2 other ML software packages.)
- Graph Dynamical Networks (GDyNets): `https://github.com/txie-93/gdynet`.

Journal Reviewer **Journal Reviewer.** Reviewed 9 articles for the following journals.

- Nature Communications (2)
- Science Advances (1)
- Journal of the American Chemical Society (1)
- Physical Review B (3)
- npj Computational Materials (1)
- Scientific Reports (1)

Awards

2015 David V. Ragone (1951) Endowed Fellowship.

2014 Tang Lixin Scholarship.

2013 China National Scholarship.

2012 China National Scholarship.