

Lei Sun

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Professional Appointments

- Assistant Professor** at Department of Chemistry, School of Science **Westlake University**, starting in Nov. 2021
Maria G. Mayer Fellow in Center for Nanoscale Materials **Argonne National Laboratory**, Oct. 2019 – Oct. 2021
Project: On-Chip Quantum Processors based on Molecular Electron Spin Qubits (Advisor: Tijana Rajh)
Postdoctoral Fellow in Department of Chemistry **Northwestern University**, Sep. 2017 – Aug. 2019
Project: Quantum Computation based on Molecular Electron Spin Qubits (Advisor: Danna E. Freedman)

Education

- Ph.D.** in Inorganic Chemistry **Massachusetts Institute of Technology**, Jun. 2017
Thesis Title: Electrical Conduction in Metal–Organic Frameworks (Advisor: Mircea Dincă)
Master in Computer Science **Georgia Institute of Technology**, Aug. 2019 – now
Specialization: Computer Perception and Robotics, Machine Learning
B.Sc. in Chemistry (Advisor: Jinglin Zuo) **Nanjing University**, Jun. 2011
Visiting Scholar (Advisor: Kim R. Dunbar) **Texas A&M University, College Station**, Jul. – Aug., 2009 & Jul. – Sep., 2010

Awards and Honors

- (1) Maria Goeppert Mayer Fellowship – Argonne National Laboratory **2019**
- (2) Chinese Government Award for Outstanding Self-Financed Student Abroad **2017**
- (3) Dreyfus Environmental Postdoctoral Fellowship – Northwestern University **2017**
- (4) Davison Thesis Prize (Best Inorganic Chemistry Thesis) – Massachusetts Institute of Technology **2017**
- (5) Teaching Assistant Award in Department of Chemistry – Massachusetts Institute of Technology **2012**
- (6) Davison Fellowship – Massachusetts Institute of Technology **2011**
- (7) Jiang Wenruo Honors Scholarship – Nanjing University **2010**
- (8) National Scholarship – Nanjing University **2009**
- (9) Tung OOCL Scholarship – Nanjing University **2008**
- (10) First Prize, 20th National Chemistry Olympiad, China **2007**

Invited Presentations

- (1) **Sun, L.**; Tulchinsky, Y.; Hendon, C. H.; Park, S. S.; Wang, F.; Dincă, M. "Octahedrally-Coordinated Fe(II) Optimizes Electrical Conductivity of Metal–Organic Frameworks" *MOF 2016: 5th International Conference on Metal-Organic Frameworks & Open Framework Compounds*, Long Beach, California, USA, Sep. 11–15, 2016 (oral presentation).
- (2) **Sun, L.**; Liao, B.; Sheberla, D.; Kraemer, D.; Zhou, J.; Jones, R.; Stach, E.; Nykypanchuk, D.; Akey, A.; Stavila, V.; Talin, A. A.; Allendorf, M.; Chen, G.; Léonard, F.; Dincă, M. "High Thermoelectric Figure of Merit of a Two-Dimensional Metal–Organic Framework, Ni₃(hexaiminotriphenylene)₂" *Gordon Research Seminar on Solid State Chemistry*, New London, New Hampshire, USA, Jul. 16–17, 2016 (poster presentation).
- (3) **Sun, L.**; Sheberla, D.; Skorupskii, G.; Dincă, M. "Two-Dimensional Metal–Organic Frameworks: Designable Two-Dimensional Materials" *Gordon Research Conference on Two-Dimensional Electronics Beyond Graphene*, South Hadley, Massachusetts, USA, Jun. 5–10, 2016 (poster presentation).
- (4) **Sun, L.**; Miyakai, T.; Hendon, C. H.; Seki, S.; Walsh, A.; Dincă, M. "Electrically Conductive Metal–Organic Frameworks Based on Through-Bond Charge Transport Design Principle" *250th ACS Meeting*, Boston, Massachusetts, USA, Aug. 16–20,

2015 (oral presentation).

- (5) **Sun, L.**; Miyakai, T.; Seki, S.; Dincă, M. "Semiconductive Metal–Organic Frameworks Based on Charge Transport through Metal–Sulfur Chains" *Gordon Research Conference on Electron Donor-Acceptor Interactions*, Newport, Rhode Island, USA, Aug. 3–8, 2014 (poster presentation).
- (6) **Sun, L.**; Zhang, Z.; Zhao, H.; Dunbar, K. R. "Molecular Conductors Based on Ag(TCNQ) and Its Derivatives" *2nd Asian Conference on Coordination Chemistry*, Nanjing, Jiangsu, China, Nov. 1–4, 2009 (poster presentation).

Patent

Dincă, M.; Sheberla, D.; **Sun, L.**; Wade, C. "Compositions and methods comprising conductive metal–organic frameworks and uses thereof" **2014** – US Provisional Application No. 61/988, 952; 62/091, 100.

Publications

Google Scholar: <https://scholar.google.com/citations?hl=en&user=DDI1aPYAAAAJ>

ORCID: <https://orcid.org/0000-0001-8467-6750>

Previous publications

1. Austin M. Evans, Kelsey A. Collins, Sangni Xun, Taylor G. Allen, Samik Jhulki, Ioannina Castano, Hannah L. Smith, Michael J. Strauss, Alexander K. Oanta, Lujia Liu, **Lei Sun**, Obadiah G. Reid, Gjergji Sini, Danilo Puggioni, James M. Rondinelli, Tijana Rajh, Nathan C. Gianneschi, Antoine Kahn, Danna E. Freedman, Hong Li, Stephen Barlow, Garry Rumbles, Jean-Luc Brédas, Seth R. Marder, William R. Dichtel* "Controlled *n*-Doping of Naphthalene Diimide-Based Two-Dimensional Polymers" *Adv. Mater.* **2021**, doi: 10.1002/adma.202101932.
2. Yiran Wang[†], Michael E. Ziebelt[†], **Lei Sun**, J. Tyler Gish, Tyler J. Pearson, Xue-Zeng Lu, Agnes E. Thorarinsdottir, Mark C. Hersam, Jeffrey R. Long[‡], Danna E. Freedman[‡], James M. Rondinelli[‡], Danilo Puggioni[‡], T. David Harris^{*} "Strong Magnetocrystalline Anisotropy Arising from Metal–Ligand Covalency in a Metal–Organic Candidate for 2D Magnetic Order" *Chem. Mater.* **2021**, 33, 8712–8721.
3. Jinhu Dou, Maxx Q. Arguilla, Yi Luo, Jian Li, Weizhe Zhang, **Lei Sun**, Jenna L. Mancuso, Luming Yang, Tianyang Chen, Lucas R. Parent, Grigori Skorupskii, Nicole J. Libretto, Chenyue Sun, Min Chieh Yang, Phat Vinh Dip, Edward J. Brignole, Jeffrey T. Miller, Jing Kong, Christopher H. Hendon, Junliang Sun^{*}, Mircea Dincă^{*} "Atomically Precise Single-crystal Structure of Electrically Conducting 2D Metal–Organic Frameworks" *Nature Mater.* **2021**, 20, 222–228.
4. Jian Su[†], Wen He[†], Xiao-Min Li, **Lei Sun**, Hai-Ying Wang, Ye-Qian Lan^{*}, Mengning Ding^{*}, Jing-Lin Zuo^{*} "High Electrical Conductivity in a 2D MOF with Intrinsic Superprotonic Conduction and Interfacial Pseudo-capacitance" *Matter* **2020**, 2, 711–722.
5. Cong Su[†], Zongyou Yin^{†*}, Qing-Bo Yan, Zegao Wang, Hongtao Lin, **Lei Sun**, Wenshuo Xu, Tetsuya Yamada, Xiang Ji, Nobuyuki Zettsu, Katsuya Teshima, Jamie H. Warner, Mircea Dincă, Juejun Hu, Mingdong Dong, Gang Su, Jing Kong, Ju Li[‡] "Waterproof Molecular Monolayers Stabilize 2D Materials" *Proc. Natl. Acad. Sci. U. S. A.* **2019**, 116, 20844–20849.
6. Lujia Liu, Jordan A. DeGayner, **Lei Sun**, David Z. Zee, T. David Harris^{*} "Reversible Redox Switching of Magnetic Order and Electrical Conductivity in a 2D Manganese Benzoquinoid Framework" *Chem. Sci.* **2019**, 10, 4652–4661.
7. Xiaoxue Wang, Xu Zhang, **Lei Sun**, Dongwook Lee, Sunghwan Lee, Minghui Wang, Junjie Zhao, Yang Shao-Horn, Mircea Dincă, Tomás Palacios, Karen K. Gleason^{*} "High Electrical Conductivity and Carrier Mobility in oCVD PEDOT Thin Films by Engineered Crystallization and Acid Treatment" *Sci. Adv.* **2018**, 4, eaat5780.
8. **Lei Sun**, Christopher H. Hendon, Mircea Dincă^{*} "Coordination-Induced Reversible Electrical Conductivity Variation in the MOF-74 Analogue Fe₂(DSBDC)" *Dalton Trans.* **2018**, 47, 11739–11743.
9. Lilia S. Xie, **Lei Sun**, Ruomeng Wan, Sarah S. Park, Jordan A. DeGayner, Christopher H. Hendon, Mircea Dincă^{*} "Tunable Mixed-Valence Doping toward Record Electrical Conductivity in a Three-Dimensional Metal–Organic Framework" *J. Am. Chem. Soc.* **2018**, 140, 7411–7414.
10. Jin-Hu Dou, **Lei Sun**, Yicong Ge, Wenbin Li, Christopher H. Hendon, Ju Li, Sheraz Gul, Junko Yano, Eric A. Stach, Mircea Dincă^{*} "Signature of Metallic Behavior in the Metal–Organic Frameworks M₃(hexaiminobenzene)₂ (M = Ni, Cu)" *J. Am. Chem.*

Soc. **2017**, 139, 13608–13611.

11. **Lei Sun**, Bolin Liao, Dennis Sheberla, Daniel Kraemer, Jiawei Zhou, Eric A. Stach, Dmitri Zakharov, Vitalie Stavila, A. Alec Talin, Yicong Ge, Mark D. Allendorf, Gang Chen, François Léonard, Mircea Dincă* “A Microporous and Naturally Nanostructured Thermoelectric Metal–Organic Framework with Ultralow Thermal Conductivity” *Joule* **2017**, 1, 168–177.
12. **Lei Sun**, Christopher H. Hendon, Sarah S. Park, Yuri Tulchinsky, Ruomeng Wan, Fang Wang, Aron Walsh, Mircea Dincă* “Is Iron Unique in Promoting Electrical Conductivity in MOFs?” *Chem. Sci.* **2017**, 8, 4450–4457.
13. Jian Lu, I. Ozge Ozel, Carina A. Belvin, Xian Li, Grigorii Skorupskii, **Lei Sun**, Benjamin K. Ofori-Okai, Mircea Dincă, Nuh Gedik, Keith Nelson* “Rapid and Precise Determination of Zero-Field Splittings by Terahertz Time-Domain Electron Paramagnetic Resonance Spectroscopy” *Chem. Sci.* **2017**, 8, 7312–7323.
14. Jordan A. DeGayner, le-Rang Jeon, **Lei Sun**, Mircea Dincă, T. David Harris “2D Conductive Iron-Quinoid Magnets Ordering up to $T_C = 105$ K via Heterogeneous Redox Chemistry” *J. Am. Chem. Soc.* **2017**, 139, 4175–4184.
15. Wenbin Li, **Lei Sun**, Jingshan Qi, Pablo Jarillo-Herrero, Mircea Dincă*, Ju Li* “High Temperature Ferromagnetism in π -Conjugated Two-Dimensional Metal–Organic Frameworks” *Chem. Sci.* **2017**, 8, 2859–2867.
16. Menghao Wu*, Zhijun Wang, Junwei Liu, Wenbin Li, Huahua Fu, **Lei Sun**, Xin Liu, Minghu Pan, Hongming Weng, Mircea Dincă, Liang Fu, Ju Li* “Conetronics in 2D Metal–Organic Frameworks: Double/Half Dirac Cones and Quantum Anomalous Hall Effect” *2D Mater.* **2017**, 4, 015015.
17. **Lei Sun**, Sarah S. Park, Dennis Sheberla, Mircea Dincă* “Measuring and Reporting Electrical Conductivity in Metal–Organic Frameworks: Cd₂(TTFTB) as a Case Study” *J. Am. Chem. Soc.* **2016**, 138, 14772–14782.
18. le-Rang Jeon, **Lei Sun**, Bogdan Negru, Richard P. Van Duyne, Mircea Dincă, T. David Harris* “Solid-State Redox Switching of Magnetic Exchange and Electronic Conductivity in a Benzoquinoid-Bridged Mn^{II} Chain Compound” *J. Am. Chem. Soc.* **2016**, 138, 6583–6590.
19. Elise M. Miner, Tomohiro Fukushima, Dennis Sheberla, **Lei Sun**, Yogesh Surendranath, Mircea Dincă* “Electrochemical Oxygen Reduction Catalyzed by Ni₃(hexaiminotriphenylene)₂” *Nature Commun.* **2016**, 7, 10942.
20. **Lei Sun**†, Michael G. Campbell†, Mircea Dincă* “Electrically Conductive Porous Metal–Organic Frameworks” *Angew. Chem. Int. Ed.* **2016**, 55, 3566–3579; *Angew. Chem.* **2016**, 128, 3628–3642 (review).
21. Xuan Zhang, Mohamed R. Saber, Andrey P. Prosvirin, Joseph H. Reibenspies, **Lei Sun**, Maria Ballesteros-Rivas, Hanhua Zhao, Kim R. Dunbar* “Magnetic Ordering in TCNQ-Based Metal–Organic Frameworks with Host-Guest Interactions” *Inorg. Chem. Front.* **2015**, 2, 904–911.
22. **Lei Sun**, Christopher H. Hendon, Mikael A. Minier, Aron Walsh, Mircea Dincă* “Million-Fold Electrical Conductivity Enhancement in Fe₂(DEBDC) versus Mn₂(DEBDC) (E = S, O)” *J. Am. Chem. Soc.* **2015**, 137, 6164–6167.
23. Sarah S. Park, Eric R. Hontz, **Lei Sun**, Christopher H. Hendon, Aron Walsh, Troy Van Voorhis, Mircea Dincă* “Cation-Dependent Intrinsic Electrical Conductivity in Isostructural Tetrathiafulvalene-Based Microporous Metal–Organic Frameworks” *J. Am. Chem. Soc.* **2015**, 137, 1774–1777.
24. Dennis Sheberla, **Lei Sun**, Martin A. Blood-Forsythe, Süleyman Er, Casey R. Wade, Carl K. Brozek, Alán Aspuru-Guzik, Mircea Dincă* “High Electrical Conductivity in Ni₃(2,3,6,7,10,11-hexaiminotriphenylene)₂, a Semiconducting Metal–Organic Graphene Analogue” *J. Am. Chem. Soc.* **2014**, 136, 8859–8862.
25. **Lei Sun**, Tomoyo Miyakai, Shu Seki, Mircea Dincă* “Mn₂(2,5-disulfhydrylbenzene-1,4-dicarboxylate): A Microporous Metal–Organic Framework with Infinite (–Mn–S–)_∞ Chains and High Intrinsic Charge Mobility” *J. Am. Chem. Soc.* **2013**, 135, 8185–8188.
26. Jing Xiong, Gao-Nan Li, **Lei Sun**, Yi-Zhi Li, Jing-Lin Zuo*, Xiao-Zeng You “Mono- and Dinuclear Co/Ni Complexes Bearing Redox-Active Tetrathiafulvaleneacetylacetonate Ligands – Synthesis, Crystal Structures, and Properties” *Eur. J. Inorg. Chem.* **2011**, 5173–5181.
27. Jing Xiong, **Lei Sun**, Ya Liao, Gao-Nan Li, Jing-Lin Zuo*, Xiao-Zeng You “A New Optical and Electrochemical Sensor for Fluoride Ion Based on the Functionalized Boron-Dipyrromethene Dye with Tetrathiafulvalene Moiety” *Tetrahedron Letters* **2011**, 52, 6157–6161.

28. Gao-Nan Li, Jing Xiong, Ya Liao, **Lei Sun**, Yi-Zhi Li, Jing-Lin Zuo* "Synthesis, Structures, and Properties of Metal Complexes Involving π -Conjugated Tetrathiafulvalene-Pyridine Ligand" *Polyhedron* **2011**, 30, 2473–2478.
29. Gao-Nan Li, Tao Jin, **Lei Sun**, Jie Qin, Di Wen, Jing-Lin Zuo*, Xiao-Zeng You "Dinuclear Rhenium(I) Carbonyl Complexes Based on π -Conjugated Polypyridyl Ligands with Tetrathiafulvalenes: Synthesis, Crystal Structures, Properties and DFT Calculations" *J. Organomet. Chem.* **2011**, 696, 3076–3085.
30. Jing Xiong, **Lei Sun**, Ling-Chen Kang, Wei Liu, You-Xuan Zheng, Jing-Lin Zuo*, Xiao-Zeng You "Synthesis, Crystal Structures, and Characterization of Heteronuclear Complexes Based on a Versatile Ligand with Both Acetylacetonate and Bis(2-pyridyl) Units" *Inorg. Chim. Acta* **2011**, 376, 36–43.

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