

Lei Sun

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Professional Appointments

Assistant Professor at Department of Chemistry and Department of Physics **Westlake University**, since 2021
Maria G. Mayer Fellow at Center for Nanoscale Materials **Argonne National Laboratory**, 2019 – 2021
Project: On-Chip Quantum Processors based on Molecular Electron Spin Qubits (Advisor: Tijana Rajh)
Postdoctoral Fellow at Department of Chemistry **Northwestern University**, 2017 – 2019
Project: Quantum Computation based on Molecular Electron Spin Qubits (Advisor: Danna E. Freedman)
Research Assistant at Department of Chemistry **Texas A&M University, College Station**, 2009 & 2010 summer
Project: Synthesis and electrical characterization of coordination polymers (Advisor: Kim R. Dunbar)

Education

Ph.D. in Inorganic Chemistry **Massachusetts Institute of Technology**, 2017
Thesis: Electrical Conduction in Metal–Organic Frameworks (Advisor: Mircea Dincă)
M.Sc. in Computer Science **Georgia Institute of Technology**, 2022
Specialization: Machine Learning
B.Sc. in Chemistry (Advisor: Jinglin Zuo) **Nanjing University**, 2011

Awards and Honors

1. Westlake Mingzhu Talent – Hangzhou 2022
2. Maria Goeppert Mayer Fellowship – Argonne National Laboratory 2019
3. Chinese Government Award for Outstanding Self-Financed Student Abroad 2017
4. Dreyfus Environmental Postdoctoral Fellowship – Northwestern University 2017
5. Davison Thesis Prize (Best Inorganic Chemistry Thesis) – Massachusetts Institute of Technology 2017
6. Teaching Assistant Award in Department of Chemistry – Massachusetts Institute of Technology 2012
7. National Scholarship – Nanjing University 2009
8. First Prize, 20th National Chemistry Olympiad, China 2007

Oral Presentations

1. MOF2024 – Singapore, Jul. 15–19, 2024
2. Chinese Materials Conference – Shenzhen, Guangdong Province, China, Jul. 8–11, 2024
3. 34th CCS Congress, Inorganic Chemistry Frontiers – Guangzhou, Guangdong Province, China, Jun. 15–18, 2024
4. Frontiers in Framework Materials Symposium – Nanjing, Jiangsu Province, China, Jun. 6, 2024
5. Molecular Electronics Mini-Symposium – Beijing, China, Jan. 25, 2024
6. Chinese Materials Conference – Shenzhen, Guangdong Province, China, Jul. 8–10, 2023
7. ShanghaiTech University – Shanghai, China, Jul. 4, 2023
8. Institute of Chemistry, Chinese Academy of Science and Peking University – Beijing, China, Jun. 5, 2023
9. Chinese EPR/ESR Symposium 2023 – Hangzhou, Zhejiang Province, China, Apr. 15–17, 2023
10. Hangzhou Normal University – Nanjing, Jiangsu Province, China, Nov. 10, 2022
11. Nanjing University of Science and Technology – Nanjing, Jiangsu Province, China, Oct. 20, 2022
12. Nanjing University – Nanjing, Jiangsu Province, China, Oct. 18, 2022
13. 6th iConference on Magnetic Resonance – online, Sep. 27–28, 2022

14. MOF 2016 – Long Beach, California, USA, Sep. 11–15, 2016
15. 250th ACS Meeting – Boston, Massachusetts, USA, Aug. 16–20, 2015

Patent

1. Mircea Dincă, Dennis Sheberla, **Lei Sun**, Casey R. Wade “Compositions and methods comprising conductive metal–organic frameworks and uses thereof” **2014** – US Provisional Application No. 61/988, 952; 62/091, 100.

Publications

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Preprints

1. Xiya Du, **Lei Sun*** “Optimizing Spin Qubit Performance of Lanthanide-Based Metal–Organic Frameworks” *ChemRxiv* **2024**, doi: 10.26434/chemrxiv-2024-zzs16.
2. Zhichao Pan†, Xing Huang†, Yunlong Fan, Shaoze Wang, Yiyu Liu, Xuzhong Cong, Tingsong Zhang, Shichao Qi, Ying Xing, Yu-Qing Zheng, Jian Li, Xiaoming Zhang, Wei Xu, **Lei Sun**, Jian Wang, Jin-Hu Dou* “Atomic-Precision Non-van der Waals 2D Structures: Superconductivity in π -d Conjugated Coordination Polymers” *ChemRxiv* **2024**, doi: 10.26434/chemrxiv-2024-296c0.
3. Aimei Zhou, Denan Li, Mingshu Tan, Yanpei Lv, Simin Pang, Xinxing Zhao, Zhifu Shi, Jun Zhang, Feng Jin, Shi Liu, **Lei Sun*** “Phononic Modulation of Spin-Lattice Relaxation in Molecular Qubit Frameworks” *ChemRxiv* **2024**, doi: 10.26434/chemrxiv-2024-db2x4

Independent Publications

1. Yingchao Wang, Parker S. Brodale, Xiaohe Miao, Christopher H. Hendon, **Lei Sun*** “Atmospheric Modulation of Apparent Electrical Conductivity in a Metal–Organic Framework” *Commun. Mater.* **2024**, 5, 172.
2. Jiawei Qiu†, Laura Abella†, Xiya Du†, Zhengkai Cao, Zhiwen He, Qingyu Meng, Yingjing Yan, Josep M. Poblet, **Lei Sun***, Antonio Rodriguez-Fortea*, Ning Chen* “CaY@C_{2n}: Exploring Molecular Qubits with Ca–Y Metal–Metal Bond” *J. Am. Chem. Soc.* **2024**, 146, 24310–24319.
3. Xiya Du, Aimei Zhou, **Lei Sun*** “Coherent Addressing of Single Molecular Electron Spin Qubits” *Chin. J. Chem.* **2024**, 42, 2895–2901.
4. Rui-Hao Bi, Yu Su, Yao Wang, **Lei Sun**, Wenjie Dou* “Spin-Lattice Relaxation with Non-Linear Couplings: Comparison between Fermi’s Golden Rule and Extended Dissipaton Equation of Motion” *J. Chem. Phys.* **2024**, 161, 024105.
5. Aimei Zhou, Zhecheng Sun, **Lei Sun*** “Stable Organic Radical Qubits and Their Applications in Quantum Information Science” *The Innovation* **2024**, 5, 100662.
6. Shaoze Wang, Yingchao Wang, Haozhou Sun, **Lei Sun*** “Emergent Physics in Metal–Organic Frameworks” *Chin. J. Chem.* **2024**, 42, 2514–2519.
7. Jinlong Lin, Huibiao Zhang, Mojgan Asadi, Kai Zhao, Luming Yang, Yunlong Fan, Jintao Zhu, Qianyi Liu, **Lei Sun**, Wenjun Xie, Chenru Duan, Fanyang Mo, Jin-Hu Dou* “Machine Learning-Driven Discovery and Structure–Activity Relationship Analysis of Conductive Metal–Organic Frameworks” *Chem. Mater.* **2024**, 36, 5436–5445.
8. Lauren E. McNamara†, Aimei Zhou†, Tijana Rajh, **Lei Sun***, John S. Anderson* “Realizing Solution-Phase Room Temperature Quantum Coherence in a Tetrathiafulvalene-Based Diradicaloid Complex” *Cell. Rep. Phys. Sci.* **2023**, 4, 101693.

Previous Publications

1. Kathleen R. Mullin, Rianna B. Greer, Michael J. Waters, M. Jeremy Amdur, **Lei Sun**, Danna E. Freedman, James M. Rondinelli† “Detrimental Increase of Spin-Phonon Coupling in Molecular Qubits on Substrates” *ACS Appl. Mater. Interface* **2024**, 16, 40160–40169.
2. Jia-Shiang Chen†, Kasidet Jing Trerayapiwat†, **Lei Sun**†, Matthew D. Krzyaniak, Michael R. Wasielewski, Tijana Rajh, Sahar

- Sharifzadeh, Xuedan Ma* "Long-Lived Electronic Spin Qubits in Single-Walled Carbon Nanotubes" *Nat. Commun.* **2023**, *14*, 848.
- Alexander K. Oanta, Kelsey A. Collins, Austin M. Evans, Saied Md Pratik, Lyndon A. Hall, Michael J. Strauss, Seth R. Marder, Deanna M. D'Alessandro, Tijana Rajh, Danna E. Freedman, Hong Li, Jean-Luc Brédas, **Lei Sun***, William R. Dichtel* "Electronic Spin Qubit Candidates Arrayed Within Layered Two-Dimensional Polymers" *J. Am. Chem. Soc.* **2023**, *145*, 689–696.
 - Tijana Rajh*, **Lei Sun**, Shobhit Gupta, Jun Yang, Haitao Zhang, Tian Zhong* "Hyperfine Interactions and Coherent Spin Dynamics of Isotopically Purified $^{167}\text{Er}^{3+}$ in Polycrystalline Y_2O_3 " *Mater. Quantum Technol.* **2022**, *2*, 045002.
 - Lei Sun**^{†,*}, Luming Yang[†], Jin-Hu Dou, Jian Li, Grigori Skorupskii, Michael Mardini, Kong Ooi Tan, Tianyang Chen, Chenyue Sun, Julius J. Oppenheim, Robert G. Griffin, Mircea Dincă*, Tijana Rajh* "Room-Temperature Quantitative Quantum Sensing of Lithium Ions with a Radical-Embedded Metal–Organic Framework" *J. Am. Chem. Soc.* **2022**, *144*, 19008–19016.
 - M. Jeremy Amdur, Kathleen R. Mullin, Michael J. Waters, Danilo Puggioni, Michael K. Wojnar, Mingqiang Gu, **Lei Sun**, Paul H. Oyala, James M. Rondinelli, Danna E. Freedman "Chemical Control of Spin–Lattice Relaxation to Discover a Room Temperature Molecular Qubit" *Chem. Sci.* **2022**, *13*, 7034–7045.
 - Xiao Yuan*, Daniel Bibl, Kahlil Khan, **Lei Sun** "Predicting Multi-Epitope Vaccine Candidates Using Natural Language Processing and Deep Learning" *2021 IEEE 21st International Conference on Bioinformatics and Bioengineering*, doi: 10.1109/BIBE52308.2021.9635304.
 - 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.* **2022**, *34*, 2101932.
 - Yiran Wang[†], Michael E. Ziebel[†], **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.
 - 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" *Nat. Mater.* **2021**, *20*, 222–228.
 - 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.
 - 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.
 - 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.
 - 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.
 - Lei Sun**, Christopher H. Hendon, Mircea Dincă* "Coordination-Induced Reversible Electrical Conductivity Variation in the MOF-74 Analogue $\text{Fe}_2(\text{DSBDC})$ " *Dalton Trans.* **2018**, *47*, 11739–11743.
 - 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.
 - 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 $M_3(\text{hexaiminobenzene})_2$ ($M = \text{Ni, Cu}$)" *J. Am. Chem. Soc.* **2017**, *139*, 13608–13611.
18. **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.
 19. **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.
 20. 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.
 21. 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.
 22. 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.
 23. 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.
 24. **Lei Sun**, Sarah S. Park, Dennis Sheberla, Mircea Dincă* "Measuring and Reporting Electrical Conductivity in Metal–Organic Frameworks: $\text{Cd}_2(\text{TTFTB})$ as a Case Study" *J. Am. Chem. Soc.* **2016**, *138*, 14772–14782.
 25. 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.
 26. Elise M. Miner, Tomohiro Fukushima, Dennis Sheberla, **Lei Sun**, Yogesh Surendranath, Mircea Dincă* "Electrochemical Oxygen Reduction Catalyzed by $\text{Ni}_3(\text{hexaiminotriphenylene})_2$ " *Nat. Commun.* **2016**, *7*, 10942.
 27. **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).
 28. 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.
 29. **Lei Sun**, Christopher H. Hendon, Mikael A. Minier, Aron Walsh, Mircea Dincă* "Million-Fold Electrical Conductivity Enhancement in $\text{Fe}_2(\text{DEBDC})$ versus $\text{Mn}_2(\text{DEBDC})$ ($E = \text{S, O}$)" *J. Am. Chem. Soc.* **2015**, *137*, 6164–6167.
 30. 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.
 31. 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 $\text{Ni}_3(2,3,6,7,10,11\text{-hexaiminotriphenylene})_2$, a Semiconducting Metal–Organic Graphene Analogue" *J. Am. Chem. Soc.* **2014**, *136*, 8859–8862.
 32. **Lei Sun**, Tomoyo Miyakai, Shu Seki, Mircea Dincă* " $\text{Mn}_2(2,5\text{-disulfhydrylbenzene-1,4-dicarboxylate})$: A Microporous Metal–Organic Framework with Infinite $(-\text{Mn}-\text{S}-)_\infty$ Chains and High Intrinsic Charge Mobility" *J. Am. Chem. Soc.* **2013**, *135*, 8185–8188.
 33. 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.
 34. 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-Dipyromethene Dye with Tetrathiafulvalene Moiety" *Tetrahedron Lett.* **2011**, *52*, 6157–6161.

35. 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.
36. 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.
37. 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.