Ryotaro Okabe

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EDUCATION

Ph.D. in Chemistry, Massachusetts Institute of Technology, *MA, USA / Sept. 2021 – Sept. 2026*

M.S. in Engineering, Institute of Science Tokyo, *Japan / Sept. 2019 – Sept. 2021*

B.S. in Engineering, Institute of Science Tokyo, *Japan / Apr. 2016 – Sept. 2019 (Early Graduation)*

- **Courses**: Quantum mechanics, Statistical mechanics, Solid state physics, Machine learning, Group theory
- **Teaching**: Quantum Mechanics (2021), General Chemistry (2022)
- **Leadership**: APS Group on Data Science Student Representative (2026–2028); Japanese Assoc. of MIT, Treasurer (2022–2024); Sidney Pacific Graduate Residence, Officer (2022–2024); Japan–US Science Forum in Boston, Organizer (2022–2024)

EXPERIENCES

Argonne Scholar (Maria Goeppert Mayer Fellow), Argonne National Laboratory, X-ray Science Division (Sponsors: Dr. Haidan Wen, Dr. Mathew Cherukara), *IL, USA* | *Oct. 2026 – Present*

- Develop AI/agent-based methods for the analysis and design of X-ray measurements at the Advanced Photon Source.

Research Assistant, Massachusetts Institute of Technology (Advisor: Prof. Mingda Li), *MA, USA* | *Nov. 2021 – Sep. 2026*

- Developed machine learning methods to explore the structure–property relationship in materials (e.g., prediction of phonon dispersion from material structures, generating quantum material candidates).
- Developed machine learning methods to localize the radiation sources with detector arrays.

Research Intern, IBM Thomas J. Watson Research Center (Mentor: Dr. Ching-Tzu Chen), *NY, USA* | *May – Aug. 2024*

- High-throughput calculation of electrical conductance in topological interconnect materials.
- Developed machine learning methods to predict the conductance of slab materials.

Research Assistant, Institute of Science Tokyo (Advisor: Prof. Yoshitaka Ishii), *Japan* | *Oct. 2018 – Aug. 2021*

- Implemented new schemes of solid-state nuclear magnetic resonance (SSNMR) for selective signal acquisition and evaluated them through multidimensional SSNMR experiments with numerical simulations.

Research Intern, Yale University (Advisor: Prof. Charles A. Schmuttenmaer), *CT, USA* | *Jan. – Apr. 2019*

- Synthesized metal-organic frameworks (MOFs) as photosensitizers and characterized them using powder X-ray diffraction, electrochemical experiments, and time-resolved terahertz spectroscopy.

Research Intern, Rice University (Advisor: Prof. Angel A. Martí), *TX, USA* | *Aug. – Sept. 2018*

- Observed the aggregation kinetics of Amyloid beta (Aβ) protein and interactions with the metal complex.

HONORS/AWARDS

- Maria Goeppert Mayer Fellowship, Argonne National Laboratory (Argonne News) | *Oct. 2026 – Oct. 2029*
- MRS 2025 Spring Graduate Student Silver Award | *Apr. 2025*
- MRS 2025 Spring Best Poster Award | *Apr. 2025*
- IBM PhD Fellowship Award (Granted 40,000 USD) | *Sept. 2024 – Aug. 2025*
- NERSC GenAI AY2024 Resource Allocation (6,800 GPU node hours, 1,000 CPU node hours) | *Jul. 2024*
- JASSO Graduate Fellowship (Granted approx. 11,000 USD) | *Sept. 2023 – Aug. 2024*
- Heiwa Nakajima Foundation Fellowship (Granted approx. 70,000 USD) | *Sept. 2021 – Aug. 2023*
- The Best Presentation Award at Master Thesis Midterm Presentation, Tokyo Institute of Technology | *Jul. 2020*
- NMR Society of Japan Young Scientists Poster Award | *Nov. 2020*
- Nakatani Foundation Graduate Fellowship (Granted approx. 35,000 USD) | *Sept. 2019 – Aug. 2021*
- Nakatani RIES Fellowship (fully funded research internship at Rice University and Yale University) | *Aug. 2018*

SKILLS

- **Programming**: Python, CUDA, MATLAB, Git, Scripting (Bash), LaTeX, HTML, Vim, Tcl
- **Software**: Machine learning (PyTorch, TensorFlow, Scikit-learn, PyTorch Lightning, WandB, Transformers), Material simulations (ABINIT, Quantum Espresso, VASP, Wannier90, FEFF, Phonopy, Phono3py, OpenMC, Kwant), NMR simulations (SIMPSON, SpinEvolution), Linux, Origin, ChemDraw, Claude Code, Codex
- **Material characterization**: Solid-state NMR, Powder X-ray diffraction, Metal-organic framework synthesis

COMMUNITY SERVICE

- **Journal peer review**: Matter, npj Quantum Mater., Phys. Rev. Lett., Phys. Rev. Mater., Phys. Rev. A, EPJ Quantum Technol., 2026 Conference on Physics and AI (PAI26) @ Stanford
- **Session chair**: APS Global Physics Summit 2026 (MAR-J42, MAR-W27), PAI26

PUBLICATIONS

† equal contribution (co-first authors); * corresponding author.

1. **R Okabe**†*, S Kishida†*, A Chotrattanapituk, D Bollettieri, T Isogawa, Y Cheng, M Li*, and M Adachi*, "Reward misalignment as an opportunity for materials discovery," *arXiv:2611.26186*, 2026.
2. D Córdova Carrizales†, A Chotrattanapituk†, LD Davis, J Ramsey, **R Okabe**, M Cheng, and M Li, "Agentic inverse design of spatially programmed materials," *arXiv:2611.03795*, 2026.
3. T Matsunaga†, **R Okabe**†, Y Liu, Y Shigemitsu, and Y Ishii, "A theoretical framework for efficient solvent suppression in solid-state NMR: Circumventing solvent-signal refocusing by adiabatic-inversion-based dephasing," *J. Magn. Reson. 392, 108183*, 2026.
4. T Isogawa†, **R Okabe**†, N Phadetsuwannukun, M Li, and P Cappellaro, "Agentic AI for Scientific Reasoning in Autonomous Quantum Sensing Experiments," *arXiv:2607.25145*, 2026.
5. A Chotrattanapituk†, **R Okabe**†, E Rha, M Al-Hinai, E Jiang, D Pajerowski, Y Cheng, JJ Turner, and M Li, "Universal Magnetic Structure Prediction from Atomic Coordinates with Near-Experimental Accuracy," *arXiv:2605.16230*, 2026.
6. A Roy, K Shen, A MacBride, A Oladipupo, M Taskeen, W Treyde, et al. (353 authors, including **R Okabe**), I Foster, and B Blaiszik, "From Knowledge to Action: Outcomes of the 2025 Large Language Model (LLM) Hackathon for Applications in Materials Science and Chemistry," *arXiv:2605.03205*, 2026.
7. MJ Landry†, **R Okabe**†, C Fu, and M Li, "Quantum Theory of Functionally Graded Materials," *arXiv:2603.03424*, 2026.
8. M Cheng†, C Fu†, **R Okabe**†, A Chotrattanapituk†, A Boonkird, NT Hung, and M Li, "Artificial intelligence-driven approaches for materials design and discovery," *Nat. Mater. 25, 174–190*, 2026.
9. M Mandal†, E Rha†, A Chotrattanapituk†, D Cordova Carrizales†, A Lygo, KB Woller, M Cheng, **R Okabe**, G Zhu, S Kishida, K Mak, CL Fu, S Michalopoulos, C Liu, L Wu, Y Zhu, S Stemmer, and M Li, "Tuning Chiral Anomaly Signature in a Dirac Semimetal via Fast-Ion Implantation," *Nano Lett. 25, 17571–17577*, 2025.
10. A Boonkird†, M Cheng†, A Chotrattanapituk†, D Cordova Carrizales, **R Okabe**, NC Drucker, M Mandal, T Nguyen, J Yeo, V Belosevich, E Spero, C Ortiz, Q Ma, L Fu, T Palacios, F Niroui, and M Li, "Are Quantum Materials Economically and Environmentally Sustainable?" *Materials Today*, 2025.
    - Press release at MIT News.
11. **R Okabe**, M Cheng, A Chotrattanapituk, M Mandal, K Mak, D Cordova Carrizales, NT Hung, X Fu, B Han, Y Wang, W Xie, RJ Cava, TS Jaakkola, Y Cheng, and M Li, "Structural Constraint Integration in a Generative Model for the Discovery of Quantum Materials," *Nat. Mater. 25, 223–230*, 2025.
    - Press release at MIT News.
12. C Fu†, M Cheng†, NT Hung†, E Rha, Z Chen, **R Okabe**, D Cordova Carrizales, M Mandal, YQ Cheng, and M Li, "AI-driven defect engineering in advanced thermoelectric materials," *Adv. Mater. 37, 2505642*, 2025.
13. M Cheng, **R Okabe**, and M Li, "Closing the superconducting gap with AI," *Newton 1, 100093*, 2025.
14. B Han†, **R Okabe**†, A Chotrattanapituk†, M Cheng†, M Li, and Y Cheng, "AI-Powered Exploration of Molecular Vibrations, Phonons and Spectroscopy," *Digit. Discov. 4, 584–624*, 2025.
15. **R Okabe**†, Z West†, A Chotrattanapituk, M Cheng, D Cordova Carrizales, W Xie, RJ Cava, and M Li, "Large Language Model-Guided Prediction Toward Quantum Materials Synthesis," *arXiv:2410.20976*, 2024.
16. P Siriviboon†, C Fu†, M Landry†, **R Okabe**, D Cordova Carrizales, Y Wang, and M Li, "Quantum Theory of X-ray Photon Correlation Spectroscopy," *arXiv:2412.03635*, 2024.
17. NT Hung, **R Okabe**, A Chotrattanapituk, and M Li, "Universal Ensemble-Embedding Graph Neural Network for Direct Prediction of Optical Spectra from Crystal Structures," *Adv. Mater. 36, 2409175*, 2024.
    - Press release at Tohoku University Research News; Graphical Abstract.
18. **R Okabe**†, A Chotrattanapituk†, A Boonkird, N Andrejevic, X Fu, TS Jaakkola, Q Song, T Nguyen, NC Drucker, S Mu, B Liao, Y Cheng, and M Li, "Virtual Node Graph Neural Network for Full Phonon Prediction," *Nat. Comput. Sci. 4, 522–531*, 2024.
    - Journal Research Briefing; July 2024 issue Front Cover; press release at MIT News.
19. M Mandal†, A Chotrattanapituk†, K Woller, H Xu, N Mao, **R Okabe**, A Boonkird, T Nguyen, NC Drucker, T Momiki, J Li, J Kong, and M Li, "Precise Fermi-level engineering in a topological Weyl semimetal via fast ion implantation," *Appl. Phys. Rev. 11, 021429*, 2024.
    - Press release at MIT News.
20. M Cheng, **R Okabe**, A Chotrattanapituk, and M Li, "Machine Learning Detection of Majorana Zero Modes from Zero Bias Peak Measurements," *Matter 7, 2507–2520*, 2024.
21. **R Okabe**†, S Xue†, J Vavrek†, J Yu, R Pavlovsky, V Negut, B Quiter, J Cates, T Liu, B Forget, S Jegelka, G Kohse, L-W Hu, and M Li, "Tetris-Inspired Detector with Neural Network for Radiation Mapping," *Nat. Commun. 15, 3061*, 2024.
    - Press release at MIT News, Physics World, Nuclear Engineering International.
22. NC Drucker, T Nguyen, M Mandal, P Siriviboon, Y Quan, A Boonkird, **R Okabe**, F Li, K Burrage, F Funuma, M Matsuda, D Abernathy, T Williams, S Chi, F Ye, C Nelson, B Liao, P Volkov, and M Li, "Incipient Nematicity from Electron Flat Bands in a Kagome Metal," *arXiv:2401.17141*, 2024.
23. **R Okabe**, M Li, Y Iwasaki, N Regnault, C Felser, M Shirai, A Kovacs, T Schrefl, and A Hirohata, "Materials Informatics for the Development and Discovery of Future Magnetic Materials," *IEEE Magn. Lett. 14, 1–5*, 2023.

• IEEE Magnetics Letters (Volume 14) Front Cover.

24. M Mandal, NC Drucker, P Siriviboon, T Nguyen, A Boonkird, TN Lamichhane, **R Okabe**, A Chotrattanapituk, and M Li, "Topological superconductors from a materials perspective," *Chem. Mater. 35, 6184–6200*, 2023.
25. NC Drucker, T Liu, Z Chen, **R Okabe**, A Chotrattanapituk, T Nguyen, Y Wang, and M Li, "Challenges and Opportunities of Machine Learning on Neutron and X-ray Scattering," *Synchrotron Radiat. News 35, 16–20*, 2022.
26. HA Merker, H Heiberger, L Nguyen, T Liu, Z Chen, N Andrejevic, NC Drucker, **R Okabe**, Y Wang, T Smidt, and M Li, "Machine Learning Magnetism Classifiers from Atomic Coordinates," *iScience 25, 105192*, 2022.
27. T Matsunaga, **R Okabe**, and Y Ishii, "Efficient solvent suppression with adiabatic inversion for ^{1}H-detected solid-state NMR," *J. Biomol. NMR 75, 365–370*, 2021.
28. B Pattengale, JG Freeze, M Guberman-Pfeffer, **R Okabe**, S Ostresh, S Chaudhuri, VS Batista, and CA Schmuttenmaer, "A Conductive Metal-Organic Framework Photoanode," *Chem. Sci. 11, 9593–9603*, 2020.
    • Conference abstract proceedings (2022).
29. B Pattengale, J Neu, S Ostresh, G Hu, JA Spies, **R Okabe**, GW Brudvig, and CA Schmuttenmaer, "Metal-Organic Framework Photoconductivity via Time-Resolved Terahertz Spectroscopy," *J. Am. Chem. Soc. 141, 9793–9797*, 2019.

PRESENTATIONS

1. **Innovation Spotlight: Japan**, Boston, MA, USA | *May 2026*
   Invited exhibition at the STEM showcase presented by the Consul General of Japan in Boston and the Museum of Science [website]
2. **UMass Boston Physics Colloquium**, Boston, MA, USA | *Mar. 2026*
   Invited Talk: "Accelerating Quantum Material Discovery with Machine Learning: From Property Prediction to Materials Design"
3. **APS Global Physics Summit 2026**, Denver, CO, USA | *Mar. 2026*
   Tutorial 4: "Generative AI for Physics: From Models to Materials" [Session website] [Colab demo]
   Oral: "Structural Constraint Integration in a Generative Model for the Discovery of Quantum Materials"
4. **Laboratory of Atomic and Solid State Physics (LASSP) Quantum Theory Seminar**, Ithaca, NY, USA | *Oct. 2025*
   Invited Talk: "Advancing Quantum Material Discovery with Geometric Machine Learning"
5. **IMRC 2025 MRS/SMM Student Poster Award Exchange Program**, Cancún, Mexico | *Aug. 2025*
   Invited Poster: "Structural Constraint Integration in Generative Model for Discovery of Quantum Material Candidates"
6. **FT Workshop: AI-Accelerated Superconductor Discovery**, Gainesville, FL, USA | *Apr. 2025*
   Poster: "Structural Constraint Integration in Generative Model for Discovery of Quantum Material Candidates"
7. **2025 MRS Spring Meeting**, Seattle, WA, USA | *Apr. 2025*
   Award Talk & Poster: "Advancing Quantum Material Discovery through Structural Constraint Integration in Generative Models"
8. **2024 MRS Fall Meeting**, Boston, MA, USA | *Dec. 2024*
   Oral: "Structural Constraint Integration in Generative Model for Discovery of Quantum Material Candidates"
   Oral: "Large Language Model-Guided Prediction Toward Quantum Materials Synthesis"
9. **Northeast Quantum Forum 2024**, Durham, NH, USA | *Oct. 2024*
   Invited Talk: "Machine-learning assisted study of quantum material properties and quantum material discovery"
10. **Quantum Materials for Emergent Applications in Quantum Science**, Telluride, CO, USA | *June 2024*
    Invited Talk: "Structural Constraint Integration in Generative Model for Discovery of Quantum Material Candidates"
11. **Competing Orders in Quantum Materials**, New Haven, CT, USA | *Mar. 2024*
    Oral: "Advancing Quantum Material Discovery through Structural Constraint Integration in Generative Models"
12. **2024 ACS Spring Meeting**, New Orleans, LA, USA | *Mar. 2024*
    Poster: "Virtual Node Augmented Machine Learning for Material Property Prediction"
13. **2023 MRS Spring Meeting**, San Francisco, CA, USA | *Apr. 2023*
    Poster: "Virtual Node Augmented Machine Learning for Material Property Prediction"
14. **2022 MRS Fall Meeting**, Boston, MA, USA | *Nov.–Dec. 2022*
    Poster: "Machine Learning Gamma Phonons from Atomic Coordinates"
15. **2022 MRS Spring Meeting** (online) | *May 2022*
    Oral: "Application of Radiation Detection Materials for Radiation Mapping with Machine Learning"
16. **22nd International Society of Magnetic Resonance Conference** (online) | *Aug. 2021*
    Poster: "Theoretical explanation of new solvent suppression scheme with adiabatic pulse and application for solid-state NMR experiments"
17. **The 59th Annual Meeting of the NMR Society of Japan**, Gunma, Japan | *Nov. 2020*
    Poster: "Development of Suppression Pulse with Adiabatic Pulse and Application for Biological Solid-State NMR"
18. **The 58th Annual Meeting of the NMR Society of Japan**, Kanagawa, Japan | *Nov. 2019*
    Poster: "Development of Suppression Pulse with Adiabatic Pulse for Solid-State NMR Experiment"