

# Ryotaro Okabe

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## EDUCATION

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

**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

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

- 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 (A $\beta$ ) protein and interactions with the metal complex.

## HONORS/AWARDS

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- MRS2025S Graduate Student Silver Award | Apr. 2025
- MRS2025S Best Poster Award | Apr. 2025
- IBM PhD Fellowship Awards (Granted 40,000 USD) | Sept. 2024 – Aug. 2025
- NERSC GenAI AY2024 Resource Allocations (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

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- **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

## PUBLICATIONS

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1. A Chotrattanapituk<sup>†</sup>, **R Okabe**<sup>†</sup>, E Rha, M Al-Hinai, E Jiang, D Pajeroski, Y Cheng, JJ Turner, and M Li\*, “Universal Magnetic Structure Prediction from Atomic Coordinates with Near-Experimental Accuracy,” [arXiv:2605.16230, 2026](#).
2. MJ Landry<sup>†</sup>, **R Okabe**<sup>†</sup>, C Fu, M Li, “Quantum Theory of Functionally Graded Materials,” [arXiv:2603.03424, 2026](#).

3. M Cheng<sup>†</sup>, C Fu<sup>†</sup>, **R Okabe**<sup>†</sup>, A Chotrattanapituk<sup>†</sup>, A Boonkird, NT Hung and M Li, “Artificial intelligence-driven approaches for materials design and discovery,” *Nat. Mater.* **25**, 174–190, **2026**.
4. M Mandal<sup>†</sup>, E Rha<sup>†</sup>, A Chotrattanapituk<sup>†</sup>, D Cordova Carrizales<sup>†</sup>, 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, M Li, “Tuning Chiral Anomaly Signature in a Dirac Semimetal via Fast-Ion Implantation,” *Nano Lett.* **25**, 51, 17571–17577, **2025**.
5. A Boonkird<sup>†</sup>, M Cheng<sup>†</sup>, A Chotrattanapituk<sup>†</sup>, 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](#).
6. **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, M Li, " Structural Constraint Integration in a Generative Model for the Discovery of Quantum Materials," *Nat. Mater.* **2025**.
  - Press release at [MIT News](#).
7. T Matsunaga<sup>†</sup>, **R Okabe**<sup>†</sup> and Yoshitaka Ishii, “Design of efficient solvent-suppression scheme in solid-state NMR: Echo-formation mechanism and dephasing by adiabatic inversion pulses,” *submitted to J. Magn. Reson.*
8. C Fu<sup>†</sup>, M Cheng<sup>†</sup>, NT Hung<sup>†</sup>, 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**.
9. M Cheng, R Okabe, and M Li, “Closing the superconducting gap with AI,” *Newton J*, 100093, **2025**.
10. B Han<sup>†</sup>, **R Okabe**<sup>†</sup>, A Chotrattanapituk<sup>†</sup>, M Cheng<sup>†</sup>, M Li and Y Cheng, “AI-Powered Exploration of Molecular Vibrations, Phonons and Spectroscopy.” *Digit. Discov.*, **4**(3), 584-624, **2025**.
11. **R Okabe**<sup>†</sup>, Z West<sup>†</sup>, 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**.
12. P Siriviboon<sup>†</sup>, C Fu<sup>†</sup>, M Landry<sup>†</sup>, **R Okabe**, D Cordova Carrizales, Y Wang and M Li, “Quantum Theory of X-ray Photon Correlation Spectroscopy,” *arXiv:2412.03635*, **2024**.
13. 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.*, 2409175, **2024**.
  - Press release at [Tohoku University Research News](#), [Graphical Abstract](#).
14. **R Okabe**<sup>†</sup>, A Chotrattanapituk<sup>†</sup>, A Boonkird, N Andrejevic, X Fu, TS Jaakkola, Q Song, T Nguyen, NC Drucker, S Mu, B Liao, Y Cheng, 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](#).
15. M Mandal<sup>†</sup>, A Chotrattanapituk<sup>†</sup>, 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](#).
16. M Cheng, **R Okabe**, A Chotrattanapituk, M Li, “Machine Learning Detection of Majorana Zero Modes from Zero Bias Peak Measurements,” *Matter* **7**, 2507, **2024**.
17. **R Okabe**<sup>†</sup>, S Xue<sup>†</sup>, J Vavrek<sup>†</sup>, J Yu, R Pavlovsky, V Negut, B Quitter, J Cates, T Liu, B Forget, S Jegelka, G Kohse, L-W Hu, 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](#).
18. 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**
19. **R Okabe**, M Li, Y Iwasaki, N Regnault, C Felser, M Shirai, A Kovacs, T Schrefl, A Hirohata. "Materials Informatics for the Development and Discovery of Future Magnetic Materials", *IEEE Magentic Letters*, **14**, 1-5, **2023**.
  - IEEE Magnetics Letters (Volume: 14) [Front Cover](#).
20. 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**, 16, 6184–6200, **2023**.

21. NC Drucker, T Liu, Z Chen, **R Okabe**, A Chotrattanapituk, T Nguyen, Y Wang, M Li, “Challenges and Opportunities of Machine Learning on Neutron and X-ray Scattering”, *Synchrotron Radiat. News*, **35**, 16-20, **2022**.
22. HA Merker, H Heiberger, L Nguyen, T Liu, Z Chen, N Andrejevic, NC Drucker, **R Okabe**, Y Wang, T Smidt, M Li, “Machine Learning Magnetism Classifiers from Atomic Coordinates” *iScience*, **25**, 10, 105192, **2022**.
23. T Matsunaga, **R Okabe**, Y Ishii, “Efficient solvent suppression with adiabatic inversion for <sup>1</sup>H-detected solid-state NMR” *J. Biomol. NMR*, **12**, 365-370, **2024**, **2021**.
24. B Pattengale, JG Freeze, M Guberman-Pfeffer, **R Okabe**, S Ostresh, S Chaudhuri, VS Batista, CA Schmuttenmaer, “A Conductive Metal-Organic Framework Photoanode,” *Chem. Sci.* **11**, 9593–9603, **2020**.
  - [Conference abstract proceedings \(2022\)](#).
25. B Pattengale, J Neu, S Ostresh, G Hu, JA. Spies, **R Okabe**, GW Brudvig, CA Schmuttenmaer. “Metal-Organic Framework Photoconductivity via Time-Resolved Terahertz Spectroscopy,” *J. Am. Chem. Soc.* **141**, 9793–9797, **2019**.

## PRESENTATIONS

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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 | April. 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. **Competing Orders in Quantum Materials**, New Haven, CT, USA | Mar 2024  
Oral: “Advancing Quantum Material Discovery through Structural Constraint Integration in Generative Models”
9. **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”
10. **Northeast Quantum Forum 2024**, Durham, NH, USA | Oct 2024  
Invited Talk: “Machine-learning assisted study of quantum material properties and quantum material discovery”
11. **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”
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. **22<sup>nd</sup> 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 59<sup>th</sup> Annual Meeting of the NMR Society of Japan**, Gunma, Japan | Nov. 2020  
Poster Presentation: “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 Presentation: “Development of Suppression Pulse with Adiabatic Pulse for Solid-State NMR Experiment”

### **COMMUNITY SERVICE**

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- Journal Peer Review: Matter., *NPJ Quantum Mater.*, *Phys. Rev. L.*, *Phys. Rev. M.*, *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