

Ryotaro Okabe

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EDUCATION

Ph.D. in Chemistry, Massachusetts Institute of Technology, MA, USA Sept. 2021–Present

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 Assistant:** Quantum Mechanics (2021), General Chemistry (2022)
- **Leadership:** Japanese Association of MIT Treasurer (2022-2024)

EXPERIENCE

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 β) protein and interactions with the metal complex.

Honors/Awards

- MRS2025S Graduate Student Silver Award | Apr. 2025
- MRS2025S Best Poster Award | Apr. 2025
- IBM PhD Fellowship Awards | Sept. 2024 – Aug. 2025
- NERSC GenAI AY2024 Resource Allocations | Jul. 2024
- JASSO Graduate Fellowship | Sept. 2023 – Aug. 2024
- Heiwa Nakajima Foundation Fellowship | 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 Fellowship | Sept. 2019 – Aug. 2021
- Nakatani RIES Fellowship | 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
- **Material characterization:** Solid-state NMR, Powder X-ray diffraction, Metal-organic framework synthesis

PUBLICATIONS

1. **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](#).

2. M Cheng*†, C Fu†, **R Okabe**†, A Chotrattanapituk†, A Boonkird, NT Hung and M Li, “AI-driven materials design: a mini-review,” [arXiv:2502.02905, 2025](#), accepted, *Nat. Mater.* **2025**.
3. T Matsunaga†, **R Okabe**† 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.*
4. M Mandal†, E Rha†, A Chotrattanapituk†, D Cordova Carrizales†, A Lygo, KB Woller, M Cheng, R Okabe, G Zhu, K Mak, CL Fu, C Liu, L Wu, Y Zhu, S Stemmer and M Li, “Tuning Chiral Anomaly Signature in a Dirac Semimetal via Fast-Ion Implantation,” [arXiv:2507.17972, 2025](#).
5. 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,” [Advanced Materials 37, 2505642, 2025](#).
6. M Cheng, R Okabe, and M Li, “Closing the superconducting gap with AI,” [Newton 1, 100093, 2025](#).
7. B Han†, **R Okabe**†, A Chotrattanapituk†, M Cheng†, M Li and Y Cheng, “AI-Powered Exploration of Molecular Vibrations, Phonons and Spectroscopy,” [Digital Discovery, 2025](#).
8. **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](#).
9. 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](#).
10. 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](#).
11. **R Okabe**†, A Chotrattanapituk†, 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](#).
12. 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](#).
13. M Cheng, **R Okabe**, A Chotrattanapituk, M Li, “Machine Learning Detection of Majorana Zero Modes from Zero Bias Peak Measurements,” [Matter 7, 2507, 2024](#).
14. **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, 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](#).
15. 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](#)
16. **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 Magnetism Letters (Volume: 14) [Front Cover](#).
17. 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](#).
18. 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](#).
19. 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](#).
20. T Matsunaga, **R Okabe**, Y Ishii, “Efficient solvent suppression with adiabatic inversion for ¹H-detected solid-state NMR” [J. Biomol. NMR. 12, 365-370, 2024, 2021](#).

21. B Pattengale, JG Freeze, M Guberman-Pfeffer, **R Okabe**, S Ostresh, S Chaudhuri, VS Batista, CA Schmittenmaer, "A Conductive Metal-Organic Framework Photoanode," [*Chem. Sci.* 11, 9593–9603, 2020](#).
 - [Conference abstract proceedings \(2022\)](#).
22. B Pattengale, J Neu, S Ostresh, G Hu, JA. Spies, **R Okabe**, GW Brudvig, CA Schmittenmaer. "Metal-Organic Framework Photoconductivity via Time-Resolved Terahertz Spectroscopy," [*J. Am. Chem. Soc.* 141, 9793–9797, 2019](#).

PRESENTATIONS

1. **IMRC 2025 MRS/SMM Student Poster Award Exchange Program, Cancún, Mexico | Aug. 2025**
Invited talk: "Structural Constraint Integration in Generative Model for Discovery of Quantum Material Candidates"
2. **2025 MRS Spring Meeting, Seattle, WA, USA | Apr. 2025**
Graduate Student Award Talk & Poster: "Advancing Quantum Material Discovery through Structural Constraint Integration in Generative Models"
3. **Competing Orders in Quantum Materials, New Haven, CT, USA | Mar 2024**
Oral: "Advancing Quantum Material Discovery through Structural Constraint Integration in Generative Models"
4. **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"
5. **Northeast Quantum Forum 2024, Durham, NH, USA | Oct 2024**
Invited Talk: "Machine-learning assisted study of quantum material properties and quantum material discovery"
6. **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"
7. **2024 ACS Spring Meeting New Orleans, LA, USA | Mar. 2024**
Poster: "Virtual Node Augmented Machine Learning for Material Property Prediction"
8. **2023 MRS Spring Meeting San Francisco, CA, USA | Apr. 2023**
Poster: "Virtual Node Augmented Machine Learning for Material Property Prediction"
9. **2022 MRS Fall Meeting Boston, MA, USA | Nov-Dec. 2022**
Poster: "Machine Learning Gamma Phonons from Atomic Coordinates"
10. **2022 MRS Spring Meeting (online) | May. 2022**
Oral: "Application of Radiation Detection Materials for Radiation Mapping with Machine Learning"
11. **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"
12. **The 59th 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"
13. **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"