

## Atsushi Ishikawa

**Affiliation:** Institute of Science Tokyo (Tokyo Institute of Technology), School of Environment and Society, Department of Transdisciplinary Science and Engineering

**Address:** 2-12-1 Ookayama, Meguro-city, Tokyo, Japan

**E-mail:** ishikawa.a.ai@m.titech.ac.jp

**Website:** <https://ishikawa-group.github.io/en/index.html>



### Education

2007~2011, Ph.D., Engineering, Kyoto University, Japan

### Professional Career

2011.4 ~ 2013.3 Quantum Chemistry Research Institute, Post-doc

2013.4 ~ 2017.3 Waseda University, Post-doc

2017.4 ~ 2019.3 National Institute for Materials Science, Post-doc

2019.4 ~ 2023.3 National Institute for Materials Science, Senior Researcher

2023.4 ~ present Institute of Science Tokyo, Associate Professor

### Selected Publications

1. Atsushi Ishikawa, "Heterogeneous Catalyst Design by Generative Adversarial Network and First-principles Based Microkinetics", *Scientific Reports*, 12(1) (2022)
2. Atsushi Ishikawa & Yoshitaka Tateyama, "A First-Principles Microkinetics for Homogeneous-Heterogeneous Reactions: Application to Oxidative Coupling of Methane Catalyzed by Magnesium Oxide", *ACS Catalysis*, 11(5), 2691–2700 (2021)
3. Atsushi Ishikawa & Yoshitaka Tateyama, "What Is the Active Site for the Oxidative Coupling of Methane Catalyzed by MgO? A Metadynamics-Biased Ab Initio Molecular Dynamics Study", *The Journal of Physical Chemistry C*, 124(11), 6054–6062 (2020)
4. Atsushi Ishikawa, Keitaro Sodeyama, Yasuhiko Igarashi, Tomofumi Nakayama, Yoshitaka Tateyama & Masato Okada, "Machine Learning Prediction of Coordination Energies for Alkali Group Elements in Battery Electrolyte Solvents", *Physical Chemistry Chemical Physics*, 21(48), 26399–26405 (2019)
5. Atsushi Ishikawa & Yoshitaka Tateyama, "First-Principles Microkinetic Analysis of NO + CO Reactions on Rh(111) Surface toward Understanding NOx Reduction Pathways", *The Journal of Physical Chemistry C*, 122(30), 17378–17388 (2018)
6. Atsushi Ishikawa, Toshiki Doi & Hiromi Nakai, "Catalytic Performance of Ru, Os, and Rh Nanoparticles for Ammonia Synthesis: A Density Functional Theory Analysis", *Journal of Catalysis*, 357, 213–222 (2018)

### Research Interests

1. Heterogeneous Catalysis
2. Quantum chemistry
3. Chemical kinetics