Atsushi Ishikawa

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Education:

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

Experience:

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

Research Areas:

Theoretical/computational study on the catalysts, battery, fuel cells

Selective Publications:

1. Atsushi Ishikawa, "Machine-Learning Descriptor Search on the Density of States Profile of Bimetallic Alloy Systems and Comparison with the d-Band Center Theory", Journal of Computational Chemistry, 45, 19, 1682-1689 (2024)
2. Atsushi Ishikawa, "Heterogeneous Catalyst Design by Generative Adversarial Network and First-principles Based Microkinetics", Scientific Reports, 12(1) (2022)
3. 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)
4. 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)
5. 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)
6. 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)
7. 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)