## Keitaro Sodeyama

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Optimization of direct extrusion process for Nd-Fe-B magnets using active learning assisted by machine learning and Bayesian optimization. Scripta Materialia, 2022, 209, 114341.	2.6	11
2	Thermodynamic aspect of sulfur, polysulfide anion and lithium polysulfide: plausible reaction path during discharge of lithium–sulfur battery. Physical Chemistry Chemical Physics, 2021, 23, 6832-6840.	1.3	11
3	Prediction of the coefficient of linear thermal expansion for the amorphous homopolymers based on chemical structure using machine learning. Science and Technology of Advanced Materials Methods, 2021, 1, 213-224.	0.4	4
4	Thermodynamic Analysis of Li-Intercalated Graphite by First-Principles Calculations with Vibrational and Configurational Contributions. Journal of Physical Chemistry C, 2021, 125, 27891-27900.	1.5	3
5	Li-ion transport at the interface between a graphite anode and Li <sub>2</sub> CO <sub>3</sub> solid electrolyte interphase: <i>ab initio</i> molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 10764-10774.	1.3	14
6	Strategy and Issue for Li-S Batteries with High Energy Density. ECS Meeting Abstracts, 2020, MA2020-02, 3529-3529.	0.0	0
7	First-Principles Analysis for Phase Stability of Li-Intercalated Graphite in Li-Ion Battery. ECS Meeting Abstracts, 2020, MA2020-02, 119-119.	0.0	0
8	Machine learning prediction of coordination energies for alkali group elements in battery electrolyte solvents. Physical Chemistry Chemical Physics, 2019, 21, 26399-26405.	1.3	38
9	Liquid electrolyte informatics using an exhaustive search with linear regression. Physical Chemistry Chemical Physics, 2018, 20, 22585-22591.	1.3	34
10	Large-Scale First-Principles Simulation on Li-Intercalated Graphite. ECS Meeting Abstracts, 2018, , .	0.0	0
11	First-Principles Study of Electron Injection and Defects at the TiO <sub>2</sub> /CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Interface of Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2017, 8, 5840-5847.	2.1	31
12	First-principles study on the cosensitization effects of Ru and squaraine dyes on a TiO2 surface. Surface Science, 2016, 649, 66-71.	0.8	5
13	Surface Properties of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> for Perovskite Solar Cells. Accounts of Chemical Research, 2016, 49, 554-561.	7.6	145
14	First-Principles Study of Ion Diffusion in Perovskite Solar Cell Sensitizers. Journal of the American Chemical Society, 2015, 137, 10048-10051.	6.6	582
15	Possibility of NCS Group Anchor for Ru Dye Adsorption to Anatase TiO2(101) Surface: A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2015, 119, 234-241.	1.5	4
16	Acetonitrile Solution Effect on Ru N749 Dye Adsorption and Excitation at TiO <sub>2</sub> Anatase Interface. Journal of Physical Chemistry C, 2014, 118, 16863-16871.	1.5	14
17	Termination Dependence of Tetragonal CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Surfaces for Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2014, 5, 2903-2909.	2.1	320
18	Space–Charge Layer Effect at Interface between Oxide Cathode and Sulfide Electrolyte in All-Solid-State Lithium-Ion Battery. Chemistry of Materials, 2014, 26, 4248-4255.	3.2	426

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19	Substitution effects of Ru–terpyridyl complexes on photovoltaic and carrier transport properties in dye-sensitized solar cells. Journal of Materials Chemistry A, 2013, 1, 11033.	5.2	12
20	A Nearâ€Infrared <i>cis</i> â€Configured Squaraine Coâ€Sensitizer for Highâ€Efficiency Dyeâ€Sensitized Solar Cells. Advanced Functional Materials, 2013, 23, 3782-3789.	7.8	59
21	Electronic structure of acetonitrile adsorbed on the anatase TiO2 (101) surface. Chemical Physics Letters, 2013, 556, 225-229.	1.2	11
22	Protonated Carboxyl Anchor for Stable Adsorption of Ru N749 Dye (Black Dye) on a TiO2 Anatase (101) Surface. Journal of Physical Chemistry Letters, 2012, 3, 472-477.	2.1	48
23	Water Contamination Effect on Liquid Acetonitrile/TiO <sub>2</sub> Anatase (101) Interface for Durable Dye-Sensitized Solar Cell. Journal of Physical Chemistry C, 2011, 115, 19849-19855.	1.5	31