サブ課題Ｂ：エネルギーの変換・貯蔵－電気エネルギー

サブ課題代表者：杉野 修

2. 学会誌･雑誌等における論文掲載

No.	掲載した論文（発表題目）	発表者氏名	発表した場所（学会誌・雑誌等名）	発表した時期	国内・外の別	査読（有り）
1	Hydrogen adsorption on Pt(111) revisited from random phase approximation	Lei Yan, Yang Sun, Yoshiyuki Yamamoto, Shusuke Kasamatsu, Ikutaro Hamada, and Osamu Sugino	Journal of Chemical Physics	2018年10月	国外	有
2	Direct coupling of first-principles calculations with replica exchange Monte Carlo sampling of ion disorder in solids	Shusuke Kasamatsu and Osamu Sugino	Journal of Physics: Condensed matter	2019年2月	国外	有
3	First-Principles Microkinetic Analysis of NO + CO Reactions on Rh(111) Surface toward Understanding NOx Reduction Pathways	Atsushi Ishikawa, Yoshitaka Tateyama	J. Phys. Chem. C **122**, 17378-17388	2018年7月	国外	有
4	Structures, Electronic States, and Reactions at Interfaces between LiNi0.5Mn1.5O4 Cathode and Ethylene Carbonate Electrolyte: A First-Principles Study	Yukihiro Okuno, Keisuke Ushirogata, Keitaro Sodeyama, Ganes Shukri, Yoshitaka Tateyama	J. Phys. Chem. C **123**, 2267-2277	2019年1月	国外	有
5	リチウムイオン電池 Solid Electrolyte Interphase (SEI) に関する第一原理計算研究	館山佳尚	J. Comput. Chem. Jpn. **18**, 18-28	2019年2月	国内	有
6	In Situ Spectroscopic Study on the Surface Hydroxylation of Diamond Electrodes	Seiji Kasahara, Taiga Ogose, Norihito Ikemiya, Takashi Yamamoto, Keisuke Natsui, Yasuyuki Yokota, Raymond A. Wong, Shota Iizuka, Nagahiro Hoshi, Yoshitaka Tateyama, Yousoo Kim, Masashi Nakamura, Yasuaki Einaga	Anal. Chem. **91**, 4980-4986	2019年3月	国外	有

7	Microscopic Elucidation of Solid-Electrolyte Interphase (SEI) Film Formation via Atomistic Reaction Simulations: Importance of Functional Groups of Electrolyte and Intact Additive Molecules	Norio Takenaka, Masataka Nagaoka	The Chemical Record, **19**, 1-13 (2019)	2019年3月	国外	有
8	The crucial role of electron transfer from interfacial molecules in the negative potential shift of Au electrode immersed in ionic liquids	T. Inagaki, N. Takenaka, and M. Nagaoka	Physical Chemistry Chemical Physics, **20**, 29362 (2018)	2018年10月	国外	有
9	Atomistic chemical computation of Olefin polymerization reaction catalyzed by (pyridylamido)hafnium(IV) complex: Application of Red Moon simulation	K. Matsumoto, M. Takayanagi, Y. Suzuki, N. Koga, and M. Nagaoka	Journal of Computational Chemistry, **40**, 421 (2019)	2018年10月	国外	有
10	Concentration Effect of Fluoroethylene Carbonate on the Formation of Solid Electrolyte Interphase Layer in Sodium-Ion Batteries	A. Bouibes, N. Takenaka, T. Fujie, K. Kubota, S. Komaba, and M. Nagaoka	ACS Applied Materials & Interfaces, **10**, 28525 (2018)	2018年8月	国外	有
11	Red Moon methodology compatible with quantum mechanics/molecular mechanics framework: Application to solid electrolyte interphase film formation in lithium-ion battery system	T. Fujie, N. Takenaka, Y. Suzuki, and M. Nagaoka	The Journal of Chemical Physics, **149**, 044113 (2018)	2018年7月	国外	有
12	Cost-Effective Method for Free-Energy Minimization in Complex Systems with Elaborated Ab Initio Potentials	C. Bistafa, Y. Kitamura, M. T. C. Martins-Costa, M. Nagaoka, and M. F. Ruiz-López	Journal of Chemical Theory and Computation, **14**, 3262, (2018)	2018年5月	国外	有
13	Exploring the effect of pendent side chain length on the structural and mechanical properties of hydrated perfluorosulfonic acid polymer membranes by molecular dynamics simulation	A.-T. Kuo, K. Takeuchi, A. Tanaka, S. Urata, S. Okazaki, W. Shinoda	Polymer, **146**, 53-62	2018年5月	国外	有
14	Difference in molecular mechanisms governing changes in membrane properties of phospholipid bilayers induced by addition of nonionic and zwitterionic surfactants	Y. Andoh, S. Kitou, S. Okazaki	J. Mol. Liquids, **271**, 933-941	2018年9月	国外	有
15	Molecular mechanism of material deformation and failure in butadiene rubber: Insight from all-atom molecular dynamics simulation using a bond breaking potential model	R. S. Payal, K. Fujimoto, C. Jang, W. Shinoda, Y. Takei, H. Shima, K. Tsunoda, S. Okazaki	Polymer, **170**, 113-119	2019年3月	国外	有

16	Development of dissociative force field for all-atomistic molecular dynamics calculation of fracture of polymers	K. Fujimoto, R. S. Payal, T. Hattori, W. Shinoda, M. Nakagaki, S. Sakaki, S. Okazaki	J. Comp. Chem. accepted.		国外	有