

サブ課題B: エネルギーの変換・貯蔵－電気エネルギー

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1. 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・雑誌名等）	発表した時期	国内・国際 の別	査読（有り の場合○を記 入）
1	Ab-initio molecular dynamics of solvation effects on reactivity at electrified interfaces	J.A. Herron, Y. Morikawa, and M. Mavrikakis	Proc. Natl. Acad. Sci. U. S. A., 113, E4937–E4945 (2016)	2016年8月	国外	○
2	Superconcentrated electrolytes for a high-voltage lithium-ion battery	Jianhui Wang, Yuki Yamada, Keitaro Sodeyama, Ching Hua Chian, Yoshitaka Tateyama, Atsuo Yamada	Nat. Commun., 7, 12032 (2016)	2016年6月	国外	○
3	Catalytic Proton Dynamics at the Water/Solid Interface of Ceria Supported Pt Clusters	Matteo Farnesi Camellone, Fabio Negreiros Ribeiro, Lucie Szabova, Yoshitaka Tateyama, Stefano Fabris	J. Am Chem. Soc., 138, 11560–11567 (2016)	2016年7月	国外	○
4	Hydrate-melt electrolytes for high-energy-density aqueous batteries	Yuki Yamada, Kenji Usui, Keitaro Sodeyama, Seongjae Ko, Yoshitaka Tateyama, Atsuo Yamada	Nat. Energy, 13, 16129 (2016)	2016年8月	国外	○
5	The Solvation Structure of Lithium Ions in an Ether Based Electrolyte Solution from First-Principles Molecular Dynamics	Martin Callsen, Keitaro Sodeyama, Zdenek Futera, Yoshitaka Tateyama, Ikutaro Hamada	J. Phys. Chem. B, 121 (2016)	2016年12月	国外	○
6	Cation Mixing Properties toward Co Diffusion at the LiCoO ₂ Cathode/ Sulfide Electrolyte Interface in a Solid-State Battery	Jun Haruyama, Keitaro Sodeyama, Yoshitaka Tateyama	ACS Appl. Mater. Interfaces (2016)	2016年12月	国外	○
7	Enhanced Li-Ion Accessibility in MXene Titanium Carbide by Steric Chloride Termination	Satoshi Kajiyama, Lucie Szabova, Hiroki Iinuma, Akira Sugahara, Kazuma Gotoh, Keitaro Sodeyama, Yoshitaka Tateyama, Masashi Okubo, Atsuo Yamada	Adv. Energy Mater., 1601873(2017)	2017年1月	国外	○
8	An Active Site Opening Mechanism in Ion Pair of (pyridylamide) Hf(IV) Catalyst: An Associative Mechanism	K. Matsumoto, K. S. Sandhya, M. Takayanagi, N. Koga, M. Nagaoka	Organometallics, 35 (24) 4099–4105 (2016) DOI: 10.1021/acs.organomet.6b00804	2016年12月	国外	○
9	Na ⁺ Binding Is Ineffective in Forming a Primary Substrate Pocket of Thrombin	I. Kurisaki, M. Nagaoka	The Journal of Physical Chemistry B, 120 (46) 11873–11879 (2016) DOI: 10.1021/acs.jpcc.6b07827	2016年5月	国外	○

10	Formation of Reactant Complex Structure for Initiation Reaction of Lactone Ring-Opening Polymerization by Cooperation of Multiple Cyclodextrin	M.Takayanagi, S.Ito, K.Matsumoto, M.Nagaoka	The Journal of Physical Chemistry B, 120 (29) 7174-7181 (2016) DOI: 10.1021/acs.jpcc.6b04372	2016年7月	国外	○
11	Additive Effect of Fluoroethylene and Difluoroethylene Carbonates for the Solid Electrolyte Interphase Film Formation in Sodium-Ion Batteries: A Quantum Chemical Study	U.Purushotham, N.Takenaka, M.Nagaoka	RSC Advances, 6, 65232-65242 (2016) DOI: 10.1039/C6RA09560G	2016年7月	国外	○
12	Revisiting the Stereochemistry of Propylene Isotactic Polymerization Reaction Mechanism on C2 symmetric $[\text{SiH}_2(\text{Ind})_2\text{ZrCH}_3]^+$ and $[\text{SiH}_2(\text{Ind})_2\text{ZrCH}_3]^+[\text{CH}_3\text{B}(\text{C}_6\text{F}_5)_3]^-$	S.K. Sankaran, N.Koga, M.Nagaoka	Bulletin of the Chemical Society of Japan, 89 1093-1105 (2016) DOI: http://dx.doi.org/10.1246/bcsj.20160119	2016年6月	国外	○
13	The Bound Na^+ is Negative Effector for Thrombin-Substrate Stereospecific Complex Formation	I.Kurisasi, M.Takayanagi, M.Nagaoka	The Journal of Physical Chemistry B, 120 (20) 4540-4547 (2016) DOI: 10.1021/acs.jpcc.6b00976	2016年5月	国外	○
14	Evaluation of atomic pressure in the multiple time-step integration algorithm	Y Andoh, A. Yamada, N. Yoshii, S Okazaki	J. Comput. Chem.	2017年1月	国外	○
15	Detailed structural analysis of a self-assembled vesicular amphiphilic NCN-pincer Palladium complex by using wide-angle X-ray scattering and molecular dynamics calculations	G. Hamasaka, T. Muto, Y. Andoh, K. Fujimoto, K. Kato, M. Takata, S. Okazaki, Y. Uozumi	Chemistry-A European Journal	2016年12月	国外	○
16	A molecular dynamics study of local pressures and interfacial tensions of SDS micelles and dodecane droplets in water	Masahiro Kitabata, Kazushi Fujimoto, Noriyuki Yoshii, and Susumu Okazaki	J. Chem. Phys.	2016年6月	国外	○
17	Molecular Dynamics Study of the Morphology of Hydrated Perfluorosulfonic Acid Polymer Membranes	An-Tsung Kuo, Wataru Shinoda, and Susumu Okazaki	J. Phys. Chem. C, 2016, 120 (45), pp 25832-25842 DOI: 10.1021/acs.jpcc.6b08015	2016年10月	国外	○