サブ課題C:エネルギー・資源の有効利用ー化学エネルギー

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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(有りの場合〇を記入)
1	Mechanism of slow crystal growth of tetrahydrofuran clathrate hydrate	Takuma Yagasaki, Masakazu Matsumoto,Hideki Tanaka	J. Phys. Chem. C. 120, 3305—3313	2016年2月	国外	〇
2	Anomalous thermodynamic properties of Ice XVI and metastable hydrates	Takuma Yagasaki, Masakazu Matsumoto,Hideki Tanaka	Phys. Rev. B 93, 054118	2016年2月	国外	〇
3	Platinum–catalyzed reduction of amides with hydrosilanes bearing dual Si–H groups: a theoretical study of the reaction mechanism	N. Nakatani, J.–y. Hasegawa, Y. Sunada, and H. Nagashima	Dalton Transactions, 44, 19344–19356 (2015)	2015年10月	国外	〇
4	Kinetic Analysis for the Multistep Profiles of Organic Reactions: Significance of the Conformational Entropy on the Rate Constants of the Claisen Rearrangement	Y. Sumiya, Y. Nagahata, T. Komatsuzaki, T. Taketsugu, and S. Maeda	J. Phys. Chem. A, 119, 11641–11649 (2015)	2015年11月	国外	〇
5	Gold Nanoparticle Decoration of Insulating Boron Nitride Nanosheet on Inert Gold Electrode Towards an Efficient Electrocatalyst for the Reduction of Oxygen to Water	G. Elumalai, H. Noguchi, A. Lyalin, T. Taketsugu, and K. Uosaki	Electrochemistry Communications, 66 53–57 (2016)	2016年3月	国外	〇
6	Long Range Functionalization of h–BN Monolayer by Carbon Doping	M. Gao, M. Adachi, A. Lyalin, and T. Taketsugu	J. Phys. Chem. C, in press http://doi.org/10.1021/acs.jpcc.5b12706	2016年3月	国外	〇
7	Revisiting the extrapolation of correlation energies to complete basis set limit	Masaki Okoshi, Teruo Atsumi, Hiromi Nakai	J. Comput. Chem. 36, 1075 (2015)	2015年4月	国外	〇
8	A divide–and–conquer method with approximate Fermi levels for parallel computations	Takeshi Yoshikawa, Hiromi Nakai	Theor. Chem. Acc. 134, 53 (2015)	2015年4月	国外	〇
9	Accompanying coordinate expansion and recurrence relation method using a transfer relation scheme for electron repulsion integrals with high angular momenta and long contractions	Masao Hayami, Junji Seino, Hiromi Nakai	J. Chem. Phys. 142, 204110 (2015)	2015年5月	国外	〇
10	Theoretical Analysis of the Oxidation Potentials of Organic Electrolyte Solvents	Masaki Okoshi, Atsushi Ishikawa, Yoshiumi Kawamura, Hiromi Nakai	ECS Electrochem. Lett. 4, A103 (2015).	2015年7月	国外	〇
11	Theoretical Study of Extremely Long yet Stable Carbon–Carbon Bonds: Effect of Attractive C···H Interactions and Small Radical Stabilization of Diamondoids	Daeheum Cho, Yasuhiro Ikabata, Takeshi Yoshikawa, Jin Yong Lee, Hiromi Nakai	Bull. Chem. Soc. Jpn. 88, 1636 (2015)	2015年9月	国外	〇
12	分割統治型密度汎関数強束縛分子動力学(DC–DFTB–MD)法の最近の展開	西村好史、海寶丈彰、中井浩巳	J. Comput. Chem. Jpn. 14, 43 (2015)	2015年9月	国内	〇
13	Divide–and–Conquer–Type Density–Functional Tight–Binding Molecular Dynamics Simulations of Proton Diffusion in a Bulk Water System	Hiromi Nakai, Aditya Wibawa Sakti, Yoshifumi Nishimura	J. Phys. Chem. B 120, 217 (2016)	2015年12月	国外	〇

14	Efficient two-component relativistic method for large systems	Hiromi Nakai	AIP Conf. Proc. 1702, 090030 (2015)	2015年12月	国外	○
15	Contrasting mechanisms for CO_2 absorption and regeneration processes in aqueous amine solutions: Insights from density-functional tight-binding molecular dynamics simulations	Hiromi Nakai, Yoshifumi Nishimura, Takeaki Kaiho, Takahito Kubota, Hiroshi Sato	Chem. Phys. Lett. 647, 127 (2016)	2016年1月	国外	○
16	Quantum chemical approach for condensed-phase thermochemistry (III): Accurate evaluation of proton hydration energy and standard hydrogen electrode potential	Atsushi Ishikawa, Hiromi Nakai	Chem. Phys. Lett. 650, 159 (2016)	2016年3月	国外	○
17	How Can We Understand Au8 Cores and Entangled Ligands of Selenolate- and Thiolate-protected Gold Nanoclusters Au24(ER)20 and Au20(ER)16 (E = Se, S; R = Ph, Me)? A Theoretical Study	N. Takagi, K. Ishimura, M. Matsui, R. Fukuda, T. Matsui, T. Nakajima, M. Ehara, S. Sakaki	J. Am. Chem. Soc. 137, 8593-8602 (2015).	2015年6月	国外	○