Norio Takenaka

List of Publications by Year
in descending order

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34 papers	881 citations	471509 17 h-index	477307 29 g-index
35 all docs	35 docs citations	35 times ranked	963 citing authors

#	Article	IF	Citations
1	On Electrolyte-Dependent Formation of Solid Electrolyte Interphase Film in Lithium-Ion Batteries: Strong Sensitivity to Small Structural Difference of Electrolyte Molecules. Journal of Physical Chemistry C, 2014, 118, 10874-10882.	3.1	118
2	A Computational Chemical Insight into Microscopic Additive Effect on Solid Electrolyte Interphase Film Formation in Sodium-Ion Batteries: Suppression of Unstable Film Growth by Intact Fluoroethylene Carbonate. Journal of Physical Chemistry C, 2015, 119, 18046-18055.	3.1	78
3	Concentration Effect of Fluoroethylene Carbonate on the Formation of Solid Electrolyte Interphase Layer in Sodium-Ion Batteries. ACS Applied Materials & Interfaces, 2018, 10, 28525-28532.	8.0	66
4	Frontiers in Theoretical Analysis of Solid Electrolyte Interphase Formation Mechanism. Advanced Materials, 2021, 33, e2100574.	21.0	65
5	The number-adaptive multiscale QM/MM molecular dynamics simulation: Application to liquid water. Chemical Physics Letters, 2012, 524, 56-61.	2.6	53
6	Additive effect of fluoroethylene and difluoroethylene carbonates for the solid electrolyte interphase film formation in sodium-ion batteries: a quantum chemical study. RSC Advances, 2016, 6, 65232-65242.	3.6	51
7	First-Principles Study on the Peculiar Water Environment in a Hydrate-Melt Electrolyte. Journal of Physical Chemistry Letters, 2019, 10, 6301-6305.	4.6	45
8	A hybrid MC/MD reaction method with rare event-driving mechanism: Atomistic realization of 2-chlorobutane racemization process in DMF solution. Chemical Physics Letters, 2013, 583, 80-86.	2.6	43
9	Microscopic Formation Mechanism of Solid Electrolyte Interphase Film in Lithium-Ion Batteries with Highly Concentrated Electrolyte. Journal of Physical Chemistry C, 2018, 122, 2564-2571.	3.1	39
10	Rational Electrolyte Design to Form Inorganicâ€“Polymeric Interphase on Silicon-Based Anodes. ACS Energy Letters, 2021, 6, 1811-1820.	17.4	39
11	Relationship between Electric Double-Layer Structure of MXene Electrode and Its Surface Functional Groups. Chemistry of Materials, 2022, 34, 2069-2075.	6.7	28
12	Reaction path optimization and vibrational frequency analysis via ab initio QM/MM free energy gradient (FEG) method: application to isomerization process of glycine in aqueous solution. Theoretical Chemistry Accounts, 2011, 130, 215-226.	1.4	26
13	An improvement in quantum mechanical description of solute-solvent interactions in condensed systems via the number-adaptive multiscale quantum mechanical/molecular mechanical-molecular dynamics method: Application to zwitterionic glycine in aqueous solution. Journal of Chemical Physics, 2012, 137, 024501.	3.0	23
14	Kinetic square scheme in oxygen-redox battery electrodes. Energy and Environmental Science, 2022, 15, 2591-2600.	30.8	21
15	Impact of Anion Asymmetry on Local Structure and Supercooling Behavior of Water-in-Salt Electrolytes. Journal of Physical Chemistry Letters, 2020, 11, 4720-4725.	4.6	20
16	Red Moon methodology compatible with quantum mechanics/molecular mechanics framework: Application to solid electrolyte interphase film formation in lithium-ion battery system. Journal of Chemical Physics, 2018, 149, 044113.	3.0	18
17	On the Importance of Lennardâ€“Jones Parameter Calibration in QM/MM Framework: Reaction Path Tracing via Free Energy Gradient Method for Ammonia Ionization Process in Aqueous Solution. Bulletin of the Chemical Society of Japan, 2010, 83, 486-494.	3.2	17
18	Impact of cis- versus trans-Configuration of Butylene Carbonate Electrolyte on Microscopic Solid Electrolyte Interphase Formation Processes in Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 15623-15629.	8.0	17

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19	Microscopic Origin of the Solid Electrolyte Interphase Formation in Fire-Extinguishing Electrolyte: Formation of Pure Inorganic Layer in High Salt Concentration. Journal of Physical Chemistry Letters, 2019, 10, 5949-5955.	4.6	15
20	Microscopic Elucidation of Solidâ€Electrolyte Interphase (SEI) Film Formation via Atomistic Reaction Simulations: Importance of Functional Groups of Electrolyte and Intact Additive Molecules. Chemical Record, 2019, 19, 799-810.	5.8	15
21	First-Principles Study on the Cation-Dependent Electrochemical Stabilities in Li/Na/K Hydrate-Melt Electrolytes. ACS Applied Materials & Interfaces, 2020, 12, 42734-42738.	8.0	15
22	Development of advanced electrolytes in Na-ion batteries: application of the Red Moon method for molecular structure design of the SEI layer. RSC Advances, 2021, 12, 971-984.	3.6	14
23	Theoretical analysis of electrode-dependent interfacial structures on hydrate-melt electrolytes. Journal of Chemical Physics, 2020, 152, 124706.	3.0	11
24	Microscopic hydration mechanism in the ammonia dissolution process: Importance of the solute QM polarization. Chemical Physics Letters, 2010, 485, 119-123.	2.6	10
25	Dual Approach to Vibrational Spectra in Solution: Microscopic Influence of Hydrogen Bonding to the State of Motion of Glycine in Water. Journal of Chemical Theory and Computation, 2014, 10, 3369-3379.	5.3	7
26	An optimum strategy for solution chemistry using semiempirical molecular orbital method: Importance of description of charge distribution. Journal of Computational Chemistry, 2010, 31, 1287-1296.	3.3	4
27	Efficient Computational Research Protocol to Survey Free Energy Surface for Solution Chemical Reaction in the QM/MM Framework: The FEG-ER Methodology and Its Application to Isomerization Reaction of Glycine in Aqueous Solution. Journal of Physical Chemistry B, 2016, 120, 2001-2011.	2.6	4
28	The crucial role of electron transfer from interfacial molecules in the negative potential shift of Au electrode immersed in ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 29362-29373.	2.8	4
29	Free Energy Gradient Method and Its Recent Related Developments: Free Energy Optimization and Vibrational Frequency Analysis in Solution. Challenges and Advances in Computational Chemistry and Physics, 2015, , 219-252.	0.6	4
30	On the smoothing of free energy landscape of solute molecules in solution: A demonstration of the stability of glycine conformers via ab initio QM/MM free energy calculation. Chemical Physics Letters, 2011, 514, 261-266.	2.6	3
31	Computational Molecular Technology Toward Macroscopic Chemical Phenomena: Red Moon Methodology and Its Related Applications. , 2019, , 201-234.		3
32	Soft X-ray Emission Studies on Hydrate-Melt Electrolytes. Journal of Physical Chemistry B, 2021, 125, 11534-11539.	2.6	3
33	An optimum strategy for solution chemistry using semiempirical molecular orbital method. II. Primary importance of reproducing electrostatic interaction in the QM/MM framework. Journal of Computational Chemistry, 2010, 31, 2628-2641.	3.3	2
34	SEI Film Formation Simulation by Using Red Moon Method Combined with QM/MM Method. Journal of Computer Chemistry Japan, 2019, 18, 29-37.	0.1	0