Perla B Balbuena

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3524659/publications.pdf

Version: 2024-02-01

310	16,689	15504 65	19749 117
papers	citations	h-index	g-index

317	317	317	17283
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Solvent Degradation and Polymerization in the Li-Metal Battery: Organic-Phase Formation in Solid-Electrolyte Interphases. ACS Applied Materials & Interfaces, 2022, 14, 2817-2824.	8.0	23
2	Unveiling the interaction of reactions and phase transition during thermal abuse of Li-ion batteries. Journal of Power Sources, 2022, 522, 230881.	7.8	24
3	Hydrogen evolution reaction mechanism on Ti₃C₂ MXene revealed by in situ/operando Raman spectroelectrochemistry. Nanoscale, 2022, 14, 5068-5078.	5.6	20
4	Phthalocyanine as catalyst for rechargeable lithium-oxygen batteries. Journal of Porphyrins and Phthalocyanines, 2022, 26, 308-315.	0.8	1
5	Theoretical and experimental study of the effects of cobalt and nickel doping within IrO2 on the acidic oxygen evolution reaction. Journal of Catalysis, 2022, 408, 64-80.	6.2	10
6	Ion mobility and solvation complexes at liquidâ€“solid interfaces in dilute, high concentration, and localized high concentration electrolytes. Materials Advances, 2022, 3, 6352-6363.	5.4	6
7	(Digital Presentation) Investigating the Origin of the Large HER Overpotential of Ti₃C₂ Using in-Situ/Operando Raman Spectroelectrochemistry. ECS Meeting Abstracts, 2022, MA2022-01, 2053-2053.	0.0	0
8	(Digital Presentation) Elucidating the Charge Storage Mechanism on Ti₃C₂ MXene through in-Situ/Operando Raman Spectroelectrochemistry. ECS Meeting Abstracts, 2022, MA2022-01, 114-114.	0.0	0
9	Polysulfide reduction and Li2S phase formation in the presence of lithium metal and solid electrolyte interphase layer. Journal of Power Sources, 2021, 485, 229289.	7.8	9
10	Solvation vs. surface charge transfer: an interfacial chemistry game drives cation motion. Chemical Communications, 2021, 57, 6189-6192.	4.1	12
11	Influence of diluent concentration in localized high concentration electrolytes: elucidation of hidden diluent-Li⁺ interactions and Li⁺ transport mechanism. Journal of Materials Chemistry A, 2021, 9, 17459-17473.	10.3	28
12	Strategies towards enabling lithium metal in batteries: interphases and electrodes. Energy and Environmental Science, 2021, 14, 5289-5314.	30.8	156
13	A solid electrolyte interphase to protect the sulfurized polyacrylonitrile (SPAN) composite for Liâ€“S batteries: computational approach addressing the electrolyte/SPAN interfacial reactivity. Journal of Materials Chemistry A, 2021, 9, 7888-7902.	10.3	9
14	Localized high concentration electrolytes decomposition under electron-rich environments. Journal of Chemical Physics, 2021, 154, 104702.	3.0	11
15	(Invited) Role of the Electrolyte on Li Cation Electrodeposition and Intercalation. ECS Meeting Abstracts, 2021, MA2021-01, 174-174.	0.0	0
16	Nucleation and Growth of Solid Electrolyte Interphase on Lithium Metal Batteries. ECS Meeting Abstracts, 2021, MA2021-01, 449-449.	0.0	0
17	Sulfurized Polyacrylonitrile (SPAN): Changes in Mechanical Properties during Electrochemical Lithiation. Journal of Physical Chemistry C, 2021, 125, 13185-13194.	3.1	5
18	Highly Reversible Aqueous Zinc Batteries enabled by Zincophilicâ€“Zincophobic Interfacial Layers and Interrupted Hydrogenâ€Bond Electrolytes. Angewandte Chemie - International Edition, 2021, 60, 18845-18851.	13.8	150

#	Article	IF	Citations
19	Highly Reversible Aqueous Zinc Batteries enabled by Zincophilicâ€“Zincophobic Interfacial Layers and Interrupted Hydrogenâ€Bond Electrolytes. Angewandte Chemie, 2021, 133, 18993-18999.	2.0	11
20	Surface microenvironment engineering of black V2O5 nanostructures for visible light photodegradation of methylene blue. Journal of Alloys and Compounds, 2021, 871, 159615.	5.5	26
21	The passivity of lithium electrodes in liquid electrolytes for secondary batteries. Nature Reviews Materials, 2021, 6, 1036-1052.	48.7	201
22	Liquid state properties of SEI components in dimethoxyethane. Journal of Chemical Physics, 2021, 155, 124701.	3.0	1
23	Enhancing Hydrogen Evolution Activity of Monolayer Molybdenum Disulfide via a Molecular Proton Mediator. ACS Catalysis, 2021, 11, 12159-12169.	11.2	19
24	Localized High Concentration Electrolyte and Its Effects on Polysulfide Structure in Solution. Journal of Physical Chemistry C, 2021, 125, 20157-20170.	3.1	16
25	Role of Polysulfide Anions in Solid-Electrolyte Interphase Formation at the Lithium Metal Surface in Liâ€“S Batteries. Journal of Physical Chemistry Letters, 2021, 12, 9360-9367.	4.6	13
26	On the role of surface oxygen during nascent single-walled carbon nanotube cap spreading and tube nucleation on iron catalysts. Carbon, 2021, 184, 470-478.	10.3	6
27	Combined density functional theory/kinetic Monte Carlo investigation of surface morphology during cycling of Li-Cu electrodes. Electrochimica Acta, 2021, 397, 139272.	5.2	3
28	Large areal capacity and dendrite-free anodes with long lifetime enabled by distributed lithium plating with mossy manganese oxides. Journal of Materials Chemistry A, 2021, 9, 9291-9300.	10.3	6
29	Sulfurized Polyacrylonitrile for High-Performance Lithiumâ€“Sulfur Batteries: In-Depth Computational Approach Revealing Multiple Sulfurâ€™s Reduction Pathways and Hidden Li⁺ Storage Mechanisms for Extra Discharge Capacity. ACS Applied Materials & Interfaces, 2021, 13, 491-502.	8.0	16
30	Understanding Solid Electrolyte Interphase Nucleation and Growth on Lithium Metal Surfaces. Batteries, 2021, 7, 73.	4.5	3
31	Decomposition Reactivities of Carbonate Electrolyte Vs. Localized High Concentration Electrolytes on NaNiO2 Cathode Surface. ECS Meeting Abstracts, 2021, MA2021-02, 290-290.	0.0	0
32	Unravel SEI Formation on Li Metal Interfaces By Mechanistic Multi-Scale Modelling. ECS Meeting Abstracts, 2021, MA2021-02, 181-181.	0.0	1
33	Effect of Charged Surfaces, High Concentrated and Localized High Concentrated Electrolytes on Lithium Ion Solvation Complex Evolution Near the Electrode Surface. ECS Meeting Abstracts, 2021, MA2021-02, 157-157.	0.0	0
34	Methane dehydrogenation on Cu and Ni surfaces with low and moderate oxygen coverage. International Journal of Quantum Chemistry, 2020, 120, e26065.	2.0	6
35	Li2S growth on graphene: Impact on the electrochemical performance of Li-S batteries. Journal of Chemical Physics, 2020, 152, 014701.	3.0	10
36	Model systems for screening and investigation of lithium metal electrode chemistry and dendrite formation. Physical Chemistry Chemical Physics, 2020, 22, 575-588.	2.8	14

#	Article	IF	Citations
37	Elucidating Interfacial Phenomena between Solid-State Electrolytes and the Sulfur-Cathode of Lithiumâ€“Sulfur Batteries. Chemistry of Materials, 2020, 32, 360-373.	6.7	38
38	A structure and activity relationship for single-walled carbon nanotube growth confirmed by in situ observations and modeling. Nanoscale, 2020, 12, 21923-21931.	5.6	9
39	Lithium oxidation and electrolyte decomposition at Li-metal/liquid electrolyte interfaces. Journal of Materials Chemistry A, 2020, 8, 17036-17055.	10.3	28
40	Local Surface Modulation Activates Metal Oxide Electrocatalyst for Hydrogen Evolution: Synthesis, Characterization, and DFT Study of Novel Black ZnO. ACS Applied Energy Materials, 2020, 3, 10590-10599.	5.1	17
41	Calculated Reduction Potentials of Electrolyte Species in Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2020, 124, 20654-20670.	3.1	18
42	Insights into lithium ion deposition on lithium metal surfaces. Physical Chemistry Chemical Physics, 2020, 22, 21369-21382.	2.8	16
43	Effects of Solid Electrolyte Interphase Components on the Reduction of LiFSI over Lithium Metal. ChemPhysChem, 2020, 21, 1310-1317.	2.1	17
44	Computational Study of the Evolution of Ni-Based Catalysts during the Dry Reforming of Methane. Energy & Fuels, 2020, 34, 4855-4864.	5.1	22
45	Mesoscale Anatomy of Dead Lithium Formation. Journal of Physical Chemistry C, 2020, 124, 6502-6511.	3.1	31
46	Reversible Crosslinked Polymer Binder for Recyclable Lithium Sulfur Batteries with High Performance. Advanced Functional Materials, 2020, 30, 2003605.	14.9	63
47	Localized High Concentration Electrolytes for High Voltage Lithiumâ€“Metal Batteries: Correlation between the Electrolyte Composition and Its Reductive/Oxidative Stability. Chemistry of Materials, 2020, 32, 5973-5984.	6.7	97
48	Effects of charged interfaces on electrolyte decomposition at the lithium metal anode. Journal of Power Sources, 2020, 472, 228449.	7.8	41
49	LiOH Formation from Lithium Peroxide Clusters and the Role of Iodide Additive. Journal of Physical Chemistry C, 2020, 124, 10280-10287.	3.1	4
50	(Invited) Interfacial Phenomena at Electrochemical Interfaces: Insights from First Principles Simulations. ECS Meeting Abstracts, 2020, MA2020-01, 2752-2752.	0.0	0
51	Localized High Concentration Electrolytes for High Voltage Lithium-Metal Batteries: Correlation between Salt, Solvent, and Diluent Contents, and Reductive Stability of the Electrolytes. ECS Meeting Abstracts, 2020, MA2020-01, 371-371.	0.0	0
52	Controlling Reactive Battery Interfaces Using Electron-Accepting Surface Layers. ECS Meeting Abstracts, 2020, MA2020-01, 125-125.	0.0	0
53	Slow Growth Approach for Lithium Ion Deposition on Lithium Metal Anode Surfaces. ECS Meeting Abstracts, 2020, MA2020-02, 794-794.	0.0	0
54	Role of Inorganic Surface Layer on Solid Electrolyte Interphase Evolution at Li-Metal Anodes. ACS Applied Materials & Interfaces, 2019, 11, 31467-31476.	8.0	75

#	Article	IF	Citations
55	The Role of Ru in Improving the Activity of Pd toward Hydrogen Evolution and Oxidation Reactions in Alkaline Solutions. ACS Catalysis, 2019, 9, 9614-9621.	11.2	112
56	Reactivity of Cu and Co Nanoparticles Supported on Mo-Doped MgO. Industrial & Engineering Chemistry Research, 2019, 58, 18213-18222.	3.7	4
57	First-Principles Study on the Initial Oxidative Decompositions of Ethylene Carbonate on Layered Cathode Surfaces of Lithium-Ion Batteries. Journal of Physical Chemistry C, 2019, 123, 14449-14458.	3.1	18
58	Atomistic Simulations of the Reactivity of Acanthite Facets toward Cyanidation. Journal of Physical Chemistry C, 2019, 123, 11888-11898.	3.1	2
59	Synthesis, characterization, and post-synthetic modification of a micro/mesoporous zirconiumâ€“tricarboxylate metalâ€“organic framework: towards the addition of acid active sites. CrystEngComm, 2019, 21, 3014-3030.	2.6	38
60	Charge-mediated cation deposition on metallic surfaces. Journal of Materials Chemistry A, 2019, 7, 8527-8539.	10.3	13
61	Mesoscale Elucidation of Self-Discharge-Induced Performance Decay in Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2019, 11, 13326-13333.	8.0	9
62	Chemical and mechanical degradation and mitigation strategies for Si anodes. Journal of Power Sources, 2019, 419, 208-218.	7.8	32
63	Effects of Dimethyl Disulfide Cosolvent on Liâ€“S Battery Chemistry and Performance. Chemistry of Materials, 2019, 31, 2377-2389.	6.7	11
64	Antiâ€Oxygen Leaking LiCoO₂. Advanced Functional Materials, 2019, 29, 1901110.	14.9	60
65	Mechanisms of alumina growth via atomic layer deposition on nickel oxide and metallic nickel surfaces. Physical Chemistry Chemical Physics, 2019, 21, 24543-24553.	2.8	5
66	Localized high concentration electrolyte behavior near a lithiumâ€“metal anode surface. Journal of Materials Chemistry A, 2019, 7, 25047-25055.	10.3	81
67	Can Single-Walled Carbon Nanotube Diameter Be Defined by Catalyst Particle Diameter?. Journal of Physical Chemistry C, 2019, 123, 30305-30317.	3.1	17
68	Can single-walled carbon nanotube diameter be defined by catalyst particle diameter?. Journal of Physical Chemistry C, 2019, 123, .	3.1	1
69	Exploring the acid catalyzed isomerization of phenanthrene under confinement in mordenite. Microporous and Mesoporous Materials, 2018, 265, 241-249.	4.4	3
70	Evaluation of dry reforming reaction catalysts via computational screening. Catalysis Today, 2018, 312, 23-34.	4.4	8
71	Understanding Ionic Diffusion through SEI Components for Lithium-Ion and Sodium-Ion Batteries: Insights from First-Principles Calculations. Chemistry of Materials, 2018, 30, 3315-3322.	6.7	88
72	Revealing reaction mechanisms of nanoconfined Li2S: implications for lithiumâ€“sulfur batteries. Physical Chemistry Chemical Physics, 2018, 20, 11713-11721.	2.8	18

#	Article	IF	Citations
73	Synergistic Effect of Graphene Oxide for Impeding the Dendritic Plating of Li. Advanced Functional Materials, 2018, 28, 1705917.	14.9	92
74	Exploring the LiOH Formation Reaction Mechanism in Lithiumâ€“Air Batteries. Chemistry of Materials, 2018, 30, 708-717.	6.7	27
75	Formation of Multilayer Graphene Domains with Strong Sulfurâ€“Carbon Interaction and Enhanced Sulfur Reduction Zones for Lithiumâ€“Sulfur Battery Cathodes. ChemSusChem, 2018, 11, 1970-1980.	6.8	41
76	Adsorption of Carbon on Partially Oxidized Low-Index Cu Surfaces. Langmuir, 2018, 34, 1311-1320.	3.5	2
77	Fluoroethylene Carbonate as a Directing Agent in Amorphous Silicon Anodes: Electrolyte Interface Structure Probed by Sum Frequency Vibrational Spectroscopy and Ab Initio Molecular Dynamics. Nano Letters, 2018, 18, 1145-1151.	9.1	59
78	Enhanced acidity of defective MOF-808: effects of the activation process and missing linker defects. Catalysis Science and Technology, 2018, 8, 847-857.	4.1	28
79	Buildup of the Solid Electrolyte Interphase on Lithium-Metal Anodes: Reactive Molecular Dynamics Study. Journal of Physical Chemistry C, 2018, 122, 10783-10791.	3.1	44
80	Explaining the singlet complexes detected for the reaction Zr(3F)â€‰+â€‰CH3CH3 through a non-spin flip scheme. Journal of Molecular Modeling, 2018, 24, 12.	1.8	3
81	Carbon Nanotubes and Related Nanomaterials: Critical Advances and Challenges for Synthesis toward Mainstream Commercial Applications. ACS Nano, 2018, 12, 11756-11784.	14.6	388
82	Unveiling the First Nucleation and Growth Steps of Inorganic Solid Electrolyte Interphase Components. Journal of Physical Chemistry C, 2018, 122, 25858-25868.	3.1	6
83	Self-Supported Hydrous Iridiumâ€“Nickel Oxide Two-Dimensional Nanoframes for High Activity Oxygen Evolution Electrocatalysts. ACS Catalysis, 2018, 8, 10498-10520.	11.2	103
84	Investigation of the Effect of Graphene-encapsulation on the O2 Release Phenomenon from LixCoO2, Studied by In-situ Heating STEM/EELS. Microscopy and Microanalysis, 2018, 24, 1626-1627.	0.4	0
85	First-principles explorations of the electrochemical lithiation dynamics of a multilayer graphene nanosheet-based sulfurâ€“carbon composite. Journal of Materials Chemistry A, 2018, 6, 18084-18094.	10.3	11
86	Lithiumâ€Pretreated Hard Carbon as Highâ€Performance Sodiumâ€Ion Battery Anodes. Advanced Energy Materials, 2018, 8, 1801441.	19.5	105
87	First-principles calculations of oxidation potentials of electrolytes in lithiumâ€“sulfur batteries and their variations with changes in environment. Physical Chemistry Chemical Physics, 2018, 20, 18811-18827.	2.8	8
88	Elucidating mechanisms of Li plating on Li anodes of lithium-based batteries. Electrochimica Acta, 2018, 284, 485-494.	5.2	19
89	Temperature effect on the nucleation of graphene on Cu (111). RSC Advances, 2018, 8, 27825-27831.	3.6	3
90	Sigma-Holes in Battery Materials Using Iso-Electrostatic Potential Surfaces. Crystals, 2018, 8, 33.	2.2	6

#	Article	IF	Citations
91	Exploring interfacial stability of solid-state electrolytes at the lithium-metal anode surface. Journal of Power Sources, 2018, 396, 782-790.	7.8	73
92	Mesoscale Understanding of Lithium Electrodeposition for Intercalation Electrodes. Journal of Physical Chemistry C, 2018, 122, 21097-21107.	3.1	6
93	Fundamental principles of battery design. Physical Sciences Reviews, 2018, 3, .	0.8	4
94	Facet-Dependent Thermal Instability in LiCoO₂. Nano Letters, 2017, 17, 2165-2171.	9.1	99
95	Tuning the Solid Electrolyte Interphase for Selective Liâ€•and Naâ€•Ion Storage in Hard Carbon. Advanced Materials, 2017, 29, 1606860.	21.0	157
96	Revealing Charge Transport Mechanisms in Li₂S₂ for Liâ€“Sulfur Batteries. Journal of Physical Chemistry Letters, 2017, 8, 1324-1330.	4.6	56
97	Why Porous Materials Have Selective Adsorptions: A Rational Aspect from Electrodynamics. Inorganic Chemistry, 2017, 56, 2614-2620.	4.0	12
98	CO₂ Capture and Separations Using MOFs: Computational and Experimental Studies. Chemical Reviews, 2017, 117, 9674-9754.	47.7	837
99	In Situ Chemical Imaging of Solid-Electrolyte Interphase Layer Evolution in Liâ€“S Batteries. Chemistry of Materials, 2017, 29, 4728-4737.	6.7	147
100	Mesoscale Evaluation of Titanium Silicide Monolayer as a Cathode Host Material in Lithiumâ€“Sulfur Batteries. Jom, 2017, 69, 1532-1536.	1.9	5
101	Dynamics of the Lithiation and Sodiation of Silicon Allotropes: From the Bulk to the Surface. Journal of the Electrochemical Society, 2017, 164, A1644-A1650.	2.9	6
102	Direct evidence of atomic-scale structural fluctuations in catalyst nanoparticles. Journal of Catalysis, 2017, 349, 149-155.	6.2	41
103	Growth of Carbon Nanostructures on Cu Nanocatalysts. Journal of Physical Chemistry C, 2017, 121, 7232-7239.	3.1	5
104	Effects of High and Low Salt Concentration in Electrolytes at Lithiumâ€“Metal Anode Surfaces. Journal of Physical Chemistry C, 2017, 121, 182-194.	3.1	128
105	First-principles investigation of Pd3Bi as a catalyst for the oxygen reduction reaction. International Journal of Hydrogen Energy, 2017, 42, 30359-30363.	7.1	4
106	Mathematical Modeling of Electrochemical Systems at Multiple Scales in Honor of Professor John Newman. Journal of the Electrochemical Society, 2017, 164, Y13-Y13.	2.9	2
107	Phase Behavior of Methaneâ€“Ethane Mixtures in Nanopores. Industrial & Engineering Chemistry Research, 2017, 56, 11634-11643.	3.7	39
108	First-Principles Investigation of Lithium Polysulfide Structure and Behavior in Solution. Journal of Physical Chemistry C, 2017, 121, 21105-21117.	3.1	53

#	Article	IF	Citations
109	Performance evaluation of catalysts in the dry reforming reaction of methane via the ratings concept. Reaction Kinetics, Mechanisms and Catalysis, 2017, 122, 53-68.	1.7	8
110	Insights into the Li Intercalation and SEI Formation on LiSi Nanoclusters. Journal of the Electrochemical Society, 2017, 164, E3457-E3464.	2.9	10
111	Structure of Supported and Unsupported Catalytic Rh Nanoparticles: Effects on Nucleation of Single-Walled Carbon Nanotubes. Langmuir, 2017, 33, 11109-11119.	3.5	1
112	Hole Polaron Diffusion in the Final Discharge Product of Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2017, 121, 17169-17175.	3.1	15
113	Structural Dependence of the Sulfur Reduction Mechanism in Carbon-Based Cathodes for Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2017, 121, 18369-18377.	3.1	17
114	Effect of solid electrolyte interphase on the reactivity of polysulfide over lithium-metal anode. Electrochimica Acta, 2017, 258, 1320-1328.	5.2	13
115	Mesoscale Elucidation of Solid Electrolyte Interphase Layer Formation in Li-Ion Battery Anode. Journal of Physical Chemistry C, 2017, 121, 26233-26240.	3.1	38
116	Elucidating electrolyte decomposition under electron-rich environments at the lithium-metal anode. Physical Chemistry Chemical Physics, 2017, 19, 30861-30873.	2.8	65
117	Reduction of Electrolyte Components on a Coated Si Anode of Lithium-Ion Batteries. Journal of Physical Chemistry Letters, 2017, 8, 3404-3408.	4.6	13
118	In situ optical measurement of the rapid Li intercalation and deintercalation dynamics in colloidal 2D layered TiS₂nanodiscs. Nanoscale, 2016, 8, 11248-11255.	5.6	5
119	Open Framework Allotropes of Silicon: Potential Anode Materials for Na and Li-ion Batteries. Electrochimica Acta, 2016, 207, 301-307.	5.2	22
120	Evaluating silicene as a potential cathode host to immobilize polysulfides in lithiumâ€“sulfur batteries. Journal of Coordination Chemistry, 2016, 69, 2090-2105.	2.2	37
121	Influence of sp³â€“sp² Carbon Nanodomains on Metal/Support Interaction, Catalyst Durability, and Catalytic Activity for the Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2016, 8, 23260-23269.	8.0	95
122	Surface Structure and Acidity Properties of Mesoporous Silica SBA-15 Modified with Aluminum and Titanium: First-Principles Calculations. Journal of Physical Chemistry C, 2016, 120, 18105-18114.	3.1	21
123	Ethylene Carbonate Reduction on Lithiated Surfaces of Hydroxylated Amorphous Silicon Dioxide. Journal of the Electrochemical Society, 2016, 163, A2197-A2202.	2.9	7
124	Scaling Atomic Partial Charges of Carbonate Solvents for Lithium Ion Solvation and Diffusion. Journal of Chemical Theory and Computation, 2016, 12, 5709-5718.	5.3	64
125	Elucidating Oligomer-Surface and Oligomer-Oligomer Interactions at a Lithiated Silicon Surface. Electrochimica Acta, 2016, 220, 312-321.	5.2	9
126	Catalytic Upgrading of Methane to Higher Hydrocarbon in a Nonoxidative Chemical Conversion. Energy & Fuels, 2016, 30, 2584-2593.	5.1	26

#	Article	IF	Citations
127	Long-Chain Polysulfide Retention at the Cathode of Liâ€“S Batteries. Journal of Physical Chemistry C, 2016, 120, 4296-4305.	3.1	85
128	Towards Next Generation Lithium-Sulfur Batteries: Non-Conventional Carbon Compartments/Sulfur Electrodes and Multi-Scale Analysis. Journal of the Electrochemical Society, 2016, 163, A730-A741.	2.9	43
129	Li₂S Film Formation on Lithium Anode Surface of Liâ€“S batteries. ACS Applied Materials & Interfaces, 2016, 8, 4700-4708.	8.0	70
130	Response of Metal Sites toward Water Effects on Postcombustion CO₂ Capture in Metalâ€“Organic Frameworks. ACS Sustainable Chemistry and Engineering, 2016, 4, 2387-2394.	6.7	24
131	Stability of Solid Electrolyte Interphase Components on Lithium Metal and Reactive Anode Material Surfaces. Journal of Physical Chemistry C, 2016, 120, 6302-6313.	3.1	139
132	Effects of oxygen coverage, catalyst size, and core composition on Pt-alloy coreâ€“shell nanoparticles for oxygen reduction reaction. Catalysis Science and Technology, 2016, 6, 5168-5177.	4.1	22
133	Dynamic structural changes in a single catalyst particle during single walled carbon nanotube growth. Microscopy and Microanalysis, 2015, 21, 571-572.	0.4	0
134	Structure and dynamics of metallic and carburized catalytic Ni nanoparticles: effects on growth of single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2015, 17, 15056-15064.	2.8	5
135	Nanocatalyst shape and composition during nucleation of single-walled carbon nanotubes. RSC Advances, 2015, 5, 106377-106386.	3.6	15
136	Adsorption of insoluble polysulfides Li2Sx (x = 1, 2) on Li2S surfaces. Physical Chemistry Chemical Physics, 2015, 17, 9032-9039.	2.8	53
137	First-Principles Calculations of Lithiation of a Hydroxylated Surface of Amorphous Silicon Dioxide. Journal of Physical Chemistry C, 2015, 119, 16424-16431.	3.1	43
138	Structure and Reactivity of Alucone-Coated Films on Si and Li_xSi_y Surfaces. ACS Applied Materials & Interfaces, 2015, 7, 11948-11955.	8.0	39
139	Effect of the Electrolyte Composition on SEI Reactions at Si Anodes of Li-Ion Batteries. Journal of Physical Chemistry C, 2015, 119, 7060-7068.	3.1	68
140	Electronic interaction between platinum nanoparticles and nitrogen-doped reduced graphene oxide: effect on the oxygen reduction reaction. Journal of Materials Chemistry A, 2015, 3, 11891-11904.	10.3	143
141	Anisotropic Electronâ€“Phonon Coupling in Colloidal Layered TiS₂ Nanodiscs Observed via Coherent Acoustic Phonons. Journal of Physical Chemistry C, 2015, 119, 7436-7442.	3.1	11
142	Formation and Growth Mechanisms of Solid-Electrolyte Interphase Layers in Rechargeable Batteries. Chemistry of Materials, 2015, 27, 7990-8000.	6.7	225
143	Reactivity at the Lithiumâ€“Metal Anode Surface of Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2015, 119, 26828-26839.	3.1	140
144	Small-Molecule Activation Driven by Confinement Effects. ACS Catalysis, 2015, 5, 215-224.	11.2	8

#	Article	IF	Citations
145	How Impurities Affect CO₂ Capture in Metalâ€“Organic Frameworks Modified with Different Functional Groups. ACS Sustainable Chemistry and Engineering, 2015, 3, 117-124.	6.7	27
146	Electrolyte materials - Issues and challenges. AIP Conference Proceedings, 2014, , .	0.4	27
147	Activity and Durability of PEFCs Alloy Core-Shell Catalysts: Role of Surface Oxidation. Advances in Science and Technology, 2014, 93, 31-40.	0.2	1
148	Nucleation of Graphene and Its Conversion to Single-Walled Carbon Nanotubes. Nano Letters, 2014, 14, 6104-6108.	9.1	67
149	DFT Study of Reduction Mechanisms of Ethylene Carbonate and Fluoroethylene Carbonate on Li⁺-Adsorbed Si Clusters. Journal of the Electrochemical Society, 2014, 161, E3097-E3109.	2.9	36
150	Structure and Dynamics of Carbon Dioxide, Nitrogen, Water, and Their Mixtures in Metal Organic Frameworks. Journal of Chemical & Engineering Data, 2014, 59, 2973-2981.	1.9	9
151	Reduction mechanisms of additives on Si anodes of Li-ion batteries. Physical Chemistry Chemical Physics, 2014, 16, 17091-17098.	2.8	80
152	Mathematical Modeling of Electrochemical Systems at Multiple Scales. Journal of the Electrochemical Society, 2014, 161, Y9-Y9.	2.9	5
153	Dynamics of Topological Defects in Single-Walled Carbon Nanotubes during Catalytic Growth. Journal of Physical Chemistry C, 2014, 118, 4808-4817.	3.1	15
154	Modeling Electrochemical Decomposition of Fluoroethylene Carbonate on Silicon Anode Surfaces in Lithium Ion Batteries. Journal of the Electrochemical Society, 2014, 161, A213-A221.	2.9	132
155	Engineering Preferential Adsorption of Single-Walled Carbon Nanotubes on Functionalized ST-cut Surfaces of Quartz. ACS Applied Materials & Interfaces, 2014, 6, 12665-12673.	8.0	1
156	Atomic Resolution Single Walled Carbon Nanotube Nucleation Steps on Faceted Catalyst Particle Reveal Potential for Chirality Control. Microscopy and Microanalysis, 2014, 20, 1758-1759.	0.4	0
157	Spectroelectrochemical Probing of the Strong Interaction between Platinum Nanoparticles and Graphitic Domains of Carbon. ACS Catalysis, 2013, 3, 1940-1950.	11.2	78
158	Vibrational spectra of an RDX film over an aluminum substrate from molecular dynamics simulations and density functional theory. Journal of Molecular Modeling, 2013, 19, 2773-2778.	1.8	5
159	Dealloying of platinum-based alloy catalysts: Kinetic Monte Carlo simulations. Electrochimica Acta, 2013, 101, 326-333.	5.2	35
160	Experimental and theoretical study of NiMoW, NiMo, and NiW sulfide catalysts supported on an AlTiMg mixed oxide during the hydrodesulfurization of dibenzothiophene. Fuel, 2013, 113, 733-743.	6.4	44
161	Characterization of Electronic States inside Metallic Nanopores. Journal of Physical Chemistry C, 2013, 117, 18406-18413.	3.1	3
162	Building multiple adsorption sites in porous polymer networks for carbon capture applications. Energy and Environmental Science, 2013, 6, 3559.	30.8	130

#	Article	IF	Citations
163	Evolution of Structure and Activity of Alloy Electrocatalysts during Electrochemical Cycles: Combined Activity, Stability, and Modeling Analysis of PtIrCo(7:1:7) and Comparison with PtCo(1:1). Journal of Physical Chemistry C, 2013, 117, 23224-23234.	3.1	6
164	Local surface structure effect on reactivity of molecules confined between metallic surfaces. Physical Chemistry Chemical Physics, 2013, 15, 1647-1654.	2.8	9
165	Molecular dynamics simulations of metal-organic frameworks as membranes for gas mixtures separation. Journal of Membrane Science, 2013, 428, 241-250.	8.2	40
166	Characterization of carbon atomistic pathways during single-walled carbon nanotube growth on supported metal nanoparticles. Carbon, 2013, 57, 298-309.	10.3	23
167	Porous materials with pre-designed single-molecule traps for CO2 selective adsorption. Nature Communications, 2013, 4, 1538.	12.8	508
168	Water Effects on Postcombustion CO₂ Capture in Mg-MOF-74. Journal of Physical Chemistry C, 2013, 117, 3383-3388.	3.1	134
169	Understanding Activity and Durability of Core/Shell Nanocatalysts for Fuel Cells. Lecture Notes in Energy, 2013, , 589-611.	0.3	0
170	Effects of Precursor Type on the CVD Growth of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2013, 117, 10397-10409.	3.1	18
171	Characterization of Metal Nanocatalyst State and Morphology during Simulated Single-Walled Carbon Nanotube Growth. Journal of Physical Chemistry C, 2013, 117, 12061-12070.	3.1	13
172	Oxidatively stable polyaniline:polyacid electrodes for electrochemical energy storage. Physical Chemistry Chemical Physics, 2013, 15, 9654.	2.8	82
173	Preferential Adsorption of Zigzag Single-Walled Carbon Nanotubes on the ST-Cut Surface of Quartz. Journal of Physical Chemistry C, 2013, 117, 4639-4646.	3.1	3
174	Reduction Mechanisms of Ethylene Carbonate on Si Anodes of Lithium-Ion Batteries: Effects of Degree of Lithiation and Nature of Exposed Surface. ACS Applied Materials & Interfaces, 2013, 5, 13457-13465.	8.0	68
175	Effect of Subsurface Vacancies on Oxygen Reduction Reaction Activity of Pt-Based Alloys. Journal of Physical Chemistry C, 2012, 116, 14414-14422.	3.1	32
176	Window effect on CO2/N2 selectivity in metal organic framework materials. Chemical Physics Letters, 2012, 552, 136-140.	2.6	4
177	pâ€“n Junction at the Interface between Metallic Systems. Journal of Physical Chemistry Letters, 2012, 3, 818-825.	4.6	5
178	Lowâ€Energy Selective Capture of Carbon Dioxide by a Preâ€designed Elastic Singleâ€Molecule Trap. Angewandte Chemie - International Edition, 2012, 51, 9804-9808.	13.8	151
179	Evaluation of the Impact of H₂O, O₂, and SO₂ on Postcombustion CO₂ Capture in Metalâ€“Organic Frameworks. Langmuir, 2012, 28, 8064-8071.	3.5	85
180	Ethanol Reforming on Co(0001) Surfaces: A Density Functional Theory Study. Journal of Physical Chemistry A, 2012, 116, 1409-1416.	2.5	34

#	Article	IF	Citations
181	Multipoint Interactions Enhanced CO₂ Uptake: A Zeolite-like Zincâ€“Tetrazole Framework with 24-Nuclear Zinc Cages. Journal of the American Chemical Society, 2012, 134, 18892-18895.	13.7	240
182	The Structure of Benzoquinone Chemisorbed on Pd(111): Simulation of EC-STM Images and HREELS Spectra by Density Functional Theory. Electrocatalysis, 2012, 3, 353-359.	3.0	4
183	Dynamic Evolution of Supported Metal Nanocatalyst/Carbon Structure during Single-Walled Carbon Nanotube Growth. ACS Nano, 2012, 6, 720-735.	14.6	55
184	Molecular dynamics simulations of surface oxideâ€“water interactions on Pt(111) and Pt/PtCo/Pt3Co(111). Physical Chemistry Chemical Physics, 2011, 13, 20461.	2.8	14
185	Confinement-Induced Polymerization of Ethylene. Journal of Physical Chemistry C, 2011, 115, 2134-2139.	3.1	8
186	Hybrid DFT Functional-Based Static and Molecular Dynamics Studies of Excess Electron in Liquid Ethylene Carbonate. Journal of the Electrochemical Society, 2011, 158, A400.	2.9	71
187	Geometric and Electronic Confinement Effects on Catalysis. Journal of Physical Chemistry C, 2011, 115, 21324-21333.	3.1	42
188	Molecular Dynamics Simulations of Surface Oxidation on Pt(111) and Pt/PtCo/Pt₃Co(111). Journal of Physical Chemistry C, 2011, 115, 4104-4113.	3.1	23
189	Molecular Dynamics Simulations of Surface Oxidation on Pt and Pt/PtCo/Pt₃Co Nanoparticles Supported over Carbon. Journal of Physical Chemistry C, 2011, 115, 23768-23777.	3.1	19
190	Effect of the Metalâ^'Substrate Interaction Strength on the Growth of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2011, 115, 7668-7675.	3.1	20
191	Confinement-induced changes in magnetic behavior of a Ti monolayer on Pt. Chemical Physics Letters, 2011, 507, 117-121.	2.6	7
192	Kinetics and mechanism of hydrogenation of furfural on Cu/SiO2 catalysts. Journal of Catalysis, 2011, 277, 1-13.	6.2	487
193	Carbon dioxide capture-related gas adsorption and separation in metal-organic frameworks. Coordination Chemistry Reviews, 2011, 255, 1791-1823.	18.8	1,805
194	Nanocatalyst structure as a template to define chirality of nascent single-walled carbon nanotubes. Journal of Chemical Physics, 2011, 134, 014705.	3.0	36
195	Evolution of a Pt (111) surface at high oxygen coverage in acid medium. Chemical Physics Letters, 2010, 498, 328-333.	2.6	15
196	Density Functional Study of Benzoquinone Sulfonate Adsorbed on a Pd(111) Electrode Surface. Electrocatalysis, 2010, 1, 159-162.	3.0	3
197	Role of Iridium in Pt-based Alloy Catalysts for the ORR: Surface Adsorption and Stabilization Studies. Journal of the Electrochemical Society, 2010, 157, B959.	2.9	35
198	Shell-anchor-core structures for enhanced stability and catalytic oxygen reduction activity. Journal of Chemical Physics, 2010, 133, 134705.	3.0	18

#	Article	IF	Citations
199	Confinement effects on alloy reactivity. Physical Chemistry Chemical Physics, 2010, 12, 12466.	2.8	8
200	Surface segregation and stability of coreâ€“shell alloy catalysts for oxygen reduction in acid medium. Physical Chemistry Chemical Physics, 2010, 12, 2209.	2.8	114
201	Theoretical Infrared and Terahertz Spectra of an RDX/Aluminum Complex. Journal of Physical Chemistry A, 2010, 114, 2284-2292.	2.5	19
202	Adsorption of Binary Gas Mixtures in Heterogeneous Carbon Predicted by Density Functional Theory: On the Formation of Adsorption Azeotropes. Langmuir, 2010, 26, 13968-13975.	3.5	9
203	Stability of Pt Monolayers on Irâ˜Co Cores with and without a Pd Interlayer. Journal of Physical Chemistry C, 2010, 114, 13055-13060.	3.1	19
204	Interplay of Catalyst Size and Metalâ˜Carbon Interactions on the Growth of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 6952-6958.	3.1	40
205	Dissolution-Resistant Coreâ˜Shell Materials for Acid Medium Oxygen Reduction Electrocatalysts. Journal of Physical Chemistry Letters, 2010, 1, 724-728.	4.6	19
206	Surface Adsorption and Stabilization Effect of Iridium in Pt-based Alloy Catalysts for PEM Fuel Cell Cathodes. ECS Transactions, 2009, 25, 1037-1044.	0.5	2
207	Surface segregation in bimetallic Pt3M (M=Fe, Co, Ni) alloys with adsorbed oxygen. Surface Science, 2009, 603, 349-353.	1.9	46
208	Surface atomic distribution and water adsorption on Ptâ€“Co alloys. Surface Science, 2009, 603, 912-920.	1.9	20
209	First principles calculation of L21+A2 coherent equilibria in the Feâ€“Alâ€“Ti system. Physica B: Condensed Matter, 2009, 404, 2845-2847.	2.7	5
210	Effects of water and electric field on atomic oxygen adsorption on Ptâ€“Co alloys. Surface Science, 2009, 603, 3239-3248.	1.9	22
211	Growth of chiral single-walled carbon nanotube caps in the presence of a cobalt cluster. Nanotechnology, 2009, 20, 215601.	2.6	18
212	Effects of Confinement on Oxygen Adsorbed between Pt(111) Surfaces. Journal of Physical Chemistry C, 2009, 113, 7851-7856.	3.1	14
213	Carbon Adsorption and Absorption in the (111) L12 Fe3Al Surface. Journal of Physical Chemistry C, 2009, 113, 18321-18330.	3.1	2
214	Growth of Carbon Structures on Stepped (211)Co Surfaces. Journal of Physical Chemistry C, 2009, 113, 15658-15666.	3.1	19
215	Effect of Metal Cluster-Cap Interactions on the Catalyzed Growth of Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 698-709.	3.1	32
216	Size effect on the stability of Cuâ€“Ag nanoalloys. Molecular Simulation, 2009, 35, 785-794.	2.0	45

#	Article	IF	Citations
217	Nanotube nucleation versus carbon-catalyst adhesionâ€“Probed by molecular dynamics simulations. Journal of Chemical Physics, 2009, 131, 224501.	3.0	59
218	Surface segregation of core atoms in coreâ€“shell structures. Chemical Physics Letters, 2008, 456, 64-67.	2.6	43
219	Pt surface segregation in bimetallic Pt3M alloys: A density functional theory study. Surface Science, 2008, 602, 107-113.	1.9	202
220	Oxygen adsorption and surface segregation in (211) surfaces of Pt(shell)/M(core) and Pt3M (M=Co, Ir) alloys. Surface Science, 2008, 602, 3531-3539.	1.9	37
221	The role of cap chirality in the mechanism of growth of single-wall carbon nanotubes. Nanotechnology, 2008, 19, 485604.	2.6	37
222	Surface Properties and Dissolution Trends of Pt₃M Alloys in the Presence of Adsorbates. Journal of Physical Chemistry C, 2008, 112, 14520-14528.	3.1	99
223	Effect of Nanotube Cap on the Aromaticity of Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2008, 112, 13175-13180.	3.1	17
224	Atomic Oxygen Absorption into Pt-Based Alloy Subsurfaces. Journal of Physical Chemistry C, 2008, 112, 5057-5065.	3.1	34
225	Vibrational Spectra of Anhydrous and Monohydrated Caffeine and Theophylline Molecules and Crystals. Journal of Physical Chemistry A, 2008, 112, 10210-10219.	2.5	27
226	Effect of Nanotube Length on the Aromaticity of Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2008, 112, 3482-3488.	3.1	19
227	Pt(II) Uptake by Dendrimer Outer Pockets:â€‰ 1. Solventless Ligand Exchange Reaction. Journal of Physical Chemistry B, 2008, 112, 4172-4181.	2.6	11
228	Molecular Dynamics Simulations of H₂ Adsorption in Tetramethyl Ammonium Lithium Phthalocyanine Crystalline Structures. Journal of Physical Chemistry B, 2008, 112, 15775-15782.	2.6	4
229	Pt(II) Uptake by Dendrimer Outer Pockets:Â 2. Solvent-Mediated Complexation. Journal of Physical Chemistry B, 2008, 112, 4182-4193.	2.6	6
230	Kinetic Model of Surface Segregation in Pt-Based Alloys. Journal of Chemical Theory and Computation, 2008, 4, 1991-1995.	5.3	14
231	Chapter 1 Electrical characteristics of bulk-molecule interfaces. Theoretical and Computational Chemistry, 2007, 18, 1-33.	0.4	0
232	Absorption of Atomic Oxygen into Subsurfaces of Pt(100) and Pt(111):â€‰ Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 9877-9883.	3.1	95
233	Dendrimerâ^'Tetrachloroplatinate Precursor Interactions. 1. Hydration of Pt(II) Species and PAMAM Outer Pockets. Journal of Physical Chemistry A, 2007, 111, 932-944.	2.5	18
234	Chemical Environment Effects on the Atomic Oxygen Absorption into Pt(111) Subsurfaces. Journal of Physical Chemistry C, 2007, 111, 17388-17396.	3.1	50

#	Article	IF	Citations
235	Computational Studies of Structure and Dynamics of Clathrate Inhibitor Monomers in Solution. Industrial & Engineering Chemistry Research, 2007, 46, 131-142.	3.7	6
236	Catalytic Activity Tuning of a Biomimetic HOâ^'FeVO Oxidant for Methane Hydroxylation by Substituents on Aromatic Rings:Â Theoretical Study. Journal of Physical Chemistry B, 2007, 111, 2711-2718.	2.6	6
237	Chapter 6 Hydrogen adsorption in corannulene-based materials. Theoretical and Computational Chemistry, 2007, 18, 127-166.	0.4	6
238	Dendrimer-Tetrachloroplatinate Precursor Interactions. 2. Noncovalent Binding in PAMAM Outer Pockets. Journal of Physical Chemistry A, 2007, 111, 945-953.	2.5	17
239	Classical Molecular Dynamics of Clathrateâ^'Methaneâ^'Waterâ^'Kinetic Inhibitor Composite Systemsâ€. Journal of Physical Chemistry C, 2007, 111, 15554-15564.	3.1	33
240	Density functional theory analysis of reactivity of PtxPdy alloy clusters. Surface Science, 2007, 601, 165-171.	1.9	32
241	Theoretical analysis of reactivity on Pt(111) and Ptâ€“Pd(111) alloys. Surface Science, 2007, 601, 4786-4792.	1.9	45
242	Designing oxygen reduction catalysts: Insights from metalloenzymes. Chemical Physics Letters, 2007, 440, 130-133.	2.6	23
243	OOH dissociation on Pt clusters. Chemical Physics Letters, 2007, 447, 289-294.	2.6	13
244	Molecular dynamics study of the initial stages of catalyzed single-wall carbon nanotubes growth: force field development. Journal of Molecular Modeling, 2007, 13, 595-600.	1.8	47
245	Oxygen Reduction on Pd0.75Co0.25 (111) and Pt0.75Co0.25 (111) Surfaces:â€‰ An ab Initio Comparative Study. Journal of Chemical Theory and Computation, 2006, 2, 1388-1394.	5.3	37
246	Adsorption and Dissociation of H2O2on Pt and Ptâ^'Alloy Clusters and Surfaces. Journal of Physical Chemistry B, 2006, 110, 17452-17459.	2.6	76
247	Does the Decomposition of Peroxydicarbonates and Diacyl Peroxides Proceed in a Stepwise or Concerted Pathway?. Journal of Physical Chemistry A, 2006, 110, 2448-2454.	2.5	11
248	Dissolution of Oxygen Reduction Electrocatalysts in an Acidic Environment:Â Density Functional Theory Study. Journal of Physical Chemistry A, 2006, 110, 9783-9787.	2.5	55
249	Platinum Testbeds:â€‰ Interaction with Oxygen. Journal of Physical Chemistry A, 2006, 110, 11968-11974.	2.5	9
250	Perfluorobutane Sulfonic Acid Hydration and Interactions with O2Adsorbed on Pt3. Journal of Physical Chemistry A, 2006, 110, 4574-4581.	2.5	12
251	Structural and Reactivity Properties of Finite Length Cap-Ended Single-Wall Carbon Nanotubes. Journal of Physical Chemistry A, 2006, 110, 2771-2775.	2.5	13
252	Molecular dynamics studies of a model polymerâ€“catalystâ€“carbon interface. Electrochimica Acta, 2006, 51, 5904-5911.	5.2	45

#	Article	IF	Citations
253	Role of the Catalyst in the Growth of Single-Wall Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2006, 6, 1247-1258.	0.9	37
254	Molecular modeling studies of polymer electrolytes for power sources. Electrochimica Acta, 2005, 50, 3788-3795.	5.2	51
255	Molecular dynamics studies of phonon spectra in mono- and bimetallic nanoclusters. Surface Science, 2005, 581, 213-224.	1.9	37
256	Structural characterization of Pt nanoclusters deposited on graphite: Effects of substrate and surrounding medium. Catalysis Today, 2005, 105, 152-161.	4.4	9
257	Theoretical studies on cosolvation of Li ion and solvent reductive decomposition in binary mixtures of aliphatic carbonates. International Journal of Quantum Chemistry, 2005, 102, 724-733.	2.0	77
258	Complexation of Cu(II) Ions with the Lowest Generation Poly(amido-amine)-OH Dendrimers:â€‰ A Molecular Simulation Study. Journal of Physical Chemistry B, 2005, 109, 12480-12490.	2.6	18
259	Ab Initio Molecular Dynamics Simulations of the Oxygen Reduction Reaction on a Pt(111) Surface in the Presence of Hydrated Hydronium (H3O)+(H2O)2:Â Direct or Series Pathway?. Journal of Physical Chemistry B, 2005, 109, 14896-14907.	2.6	124
260	Potential Energy Surface Profile of the Oxygen Reduction Reaction on a Pt Cluster:Â Adsorption and Decomposition of OOH and H2O2. Journal of Chemical Theory and Computation, 2005, 1, 935-943.	5.3	60
261	Ab Initio and Classical Molecular Dynamics Studies of the Dilithium Phthalocyanine/Pyrite Interfacial Structure. Journal of the Electrochemical Society, 2005, 152, A1955.	2.9	4
262	Design of Oxygen Reduction Bimetallic Catalysts:â€‰ Ab-Initio-Derived Thermodynamic Guidelines. Journal of Physical Chemistry B, 2005, 109, 18902-18906.	2.6	175
263	Molecular dynamics simulations of cinchonidine-modified platinum in ethanol: comparisons with surface studies. Surface Science, 2004, 563, 57-73.	1.9	22
264	Complexation of the Lowest Generation Poly(amidoamine)-NH2Dendrimers with Metal Ions, Metal Atoms, and Cu(II) Hydrates:Â An ab Initio Study. Journal of Physical Chemistry B, 2004, 108, 15992-16001.	2.6	61
265	Crystalline Structure and Lithium-Ion Channel Formation in Self-Assembled Di-lithium Phthalocyanine:Â Theory and Experiments. Journal of Physical Chemistry B, 2004, 108, 4659-4668.	2.6	10
266	Combined ab Initio Quantum Mechanics and Classical Molecular Dynamics Studies of Polyphosphazene Polymer Electrolytes:Â Competitive Solvation of Li+and LiCF3SO3. Journal of Physical Chemistry B, 2004, 108, 15694-15702.	2.6	49
267	Ab Initio Study of the Lowest Energy Conformers and IR Spectra of Poly(amidoamine)-G0 Dendrimers. Journal of Physical Chemistry B, 2004, 108, 15982-15991.	2.6	39
268	Adsorption of O, OH, and H2O on Pt-Based Bimetallic Clusters Alloyed with Co, Cr, and Ni. Journal of Physical Chemistry A, 2004, 108, 6378-6384.	2.5	80
269	Roles of Proton and Electric Field in the Electroreduction of O2on Pt(111) Surfaces:Â Results of an Ab-Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2004, 108, 4376-4384.	2.6	100
270	THEORITICAL INSIGHTS INTO THE SEI COMPOSITION AND FORMATION MECHANISM: DENSITY FUNCTIONAL THEORY STUDIES. , 2004, , 227-275.		4

#	Article	IF	Citations
271	THEORETICAL STUDIES ON THE SOLVENT STRUCTURE AND ASSOCIATION PROPERTIES, AND ON THE Li-ION SOLVATION: IMPLICATIONS FOR SEI LAYER PHENOMENA. , 2004, , 365-397.		0
272	Lithium-Ion Batteries. , 2004, , .		233
273	Oxygen reduction on a platinum cluster. Chemical Physics Letters, 2003, 367, 439-447.	2.6	44
274	Structure and dynamics of graphite-supported bimetallic nanoclusters. Surface Science, 2003, 545, 163-179.	1.9	165
275	Hydrogen and Oxygen Adsorption on Rhn (n = 1â^'6) Clusters. Journal of Physical Chemistry A, 2003, 107, 10370-10380.	2.5	30
276	Adsorption and 2-Dimensional Association of Lithium Alkyl Dicarbonates on the Graphite Surface through O-Â·Â·Â·Li+Â·Â·Â·Ï€ (arene) Interactions. Journal of Physical Chemistry B, 2003, 107, 5503-5510.	2.6	16
277	Adsorbate Effects on Structure and Shape of Supported Nanoclusters:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 2003, 107, 11682-11689.	2.6	37
278	Associations of Lithium Alkyl Dicarbonates through OÂ·Â·Â·LiÂ·Â·Â·O Interactions. Journal of Physical Chemistry A, 2002, 106, 9582-9594.	2.5	34
279	Theoretical Studies To Understand Surface Chemistry on Carbon Anodes for Lithium-Ion Batteries:Â How Does Vinylene Carbonate Play Its Role as an Electrolyte Additive?. Journal of the American Chemical Society, 2002, 124, 4408-4421.	13.7	238
280	Platinum nanoclusters on graphite substrates: a molecular dynamics study. Molecular Physics, 2002, 100, 2165-2174.	1.7	55
281	Melting of Bimetallic Cuâ^'Ni Nanoclusters. Journal of Physical Chemistry B, 2002, 106, 7225-7236.	2.6	107
282	Theoretical Insights into the Reductive Decompositions of Propylene Carbonate and Vinylene Carbonate:Â Density Functional Theory Studies. Journal of Physical Chemistry B, 2002, 106, 4486-4495.	2.6	144
283	Computational Studies of the Interactions of Oxygen with Platinum Clusters. Journal of Physical Chemistry B, 2001, 105, 9943-9952.	2.6	118
284	Theoretical Studies of Proton Transfer in Water and Model Polymer Electrolyte Systems. Industrial & Engineering Chemistry Research, 2001, 40, 4789-4800.	3.7	66
285	Associations of Alkyl Carbonates:Â Intermolecular Câ^'HÂ·Â·Â·O Interactions. Journal of Physical Chemistry A, 2001, 105, 9972-9982.	2.5	87
286	Properties of Small Bimetallic Niâ^'Cu Clusters. Journal of Physical Chemistry A, 2001, 105, 7917-7925.	2.5	81
287	Theoretical Studies To Understand Surface Chemistry on Carbon Anodes for Lithium-Ion Batteries:Â Reduction Mechanisms of Ethylene Carbonate. Journal of the American Chemical Society, 2001, 123, 11708-11718.	13.7	404
288	Monte Carlo Simulation of Cuâ^'Ni Nanoclusters: Surface Segregation Studies. Langmuir, 2001, 17, 2047-2050.	3.5	55

#	Article	IF	Citations
289	Molecular Dynamics Study of Graphite/Electrolyte Interfaces. Journal of the Electrochemical Society, 2001, 148, A624.	2.9	36
290	Surface segregation in bimetallic nanoclusters: Geometric and thermodynamic effects. International Journal of Quantum Chemistry, 2001, 85, 580-591.	2.0	34
291	Theoretical studies of the reduction of ethylene carbonate. Chemical Physics Letters, 2000, 317, 421-429.	2.6	66
292	Density Functional Theory Study of Copper Clusters. Journal of Physical Chemistry B, 1999, 103, 2830-2840.	2.6	68
293	Theoretical Studies of Lithium Perchlorate in Ethylene Carbonate, Propylene Carbonate, and Their Mixtures. Journal of the Electrochemical Society, 1999, 146, 3613-3622.	2.9	122
294	An Eye for the Abstract. Science, 1999, 286, 430-432.	12.6	1
295	A Latticeâ€Gas Model Study of Lithium Intercalation in Graphite. Journal of the Electrochemical Society, 1999, 146, 3630-3638.	2.9	38
296	Binary Isosteric Heats of Adsorption in Carbon Predicted from Density Functional Theory. Langmuir, 1999, 15, 4570-4578.	3.5	12
297	Computational Studies of Lithium Intercalation in Model Graphite in the Presence of Tetrahydrofuran. Journal of the Electrochemical Society, 1998, 145, 3328-3334.	2.9	51
298	Aqueous Ion Transport Properties and Water Reorientation Dynamics from Ambient to Supercritical Conditions. Journal of Physical Chemistry B, 1998, 102, 3806-3814.	2.6	58
299	Isosteric Heats of Adsorption on Carbon Predicted by Density Functional Theory. Industrial & Engineering Chemistry Research, 1998, 37, 1159-1166.	3.7	42
300	Examination of the Approximations Used in Determining the Isosteric Heat of Adsorption from the Clausiusâ^'Clapeyron Equation. Langmuir, 1998, 14, 6323-6327.	3.5	272
301	Ion Solvation in Supercritical Water Based on an Adsorption Analogy. Journal of Physical Chemistry B, 1997, 101, 7998-8005.	2.6	48
302	Continuum Electrostatics Model for Ion Solvation and Relative Acidity of HCl in Supercritical Water. Journal of the American Chemical Society, 1996, 118, 6746-6752.	13.7	36
303	DFT Study of Nickel: Towards the MD Simulation of the Nickel-Water Interface. Theoretical and Computational Chemistry, 1996, 4, 649-677.	0.4	1
304	Density functional theory: Further applications. Theoretical and Computational Chemistry, 1995, 2, 383-401.	0.4	0
305	Molecular simulation of a chemical reaction in supercritical water. Journal of the American Chemical Society, 1994, 116, 2689-2690.	13.7	68
306	Theoretical interpretation of adsorption behavior of simple fluids in slit pores. Langmuir, 1993, 9, 1801-1814.	3.5	238

#	Article	IF	Citations
307	Correlation of solubilities of caffeine in supercritical solvents using a lattice model.. Journal of Chemical Engineering of Japan, 1993, 26, 323-325.	0.6	0
308	Classification of adsorption behavior: simple fluids in pores of slit-shaped geometry. Fluid Phase Equilibria, 1992, 76, 21-35.	2.5	59
309	Supercritical phase behaviour: Description of the solubility of binary solid mixtures in a supercritical solvent with a lattice gas model. Fluid Phase Equilibria, 1991, 62, 225-238.	2.5	12
310	Ion motion and charge transfer through a solid-electrolyte interphase: an atomistic view. Journal of Solid State Electrochemistry, 0, , .	2.5	1