Perla B Balbuena

List of Publications by Year
in descending order

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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	Carbon dioxide capture-related gas adsorption and separation in metal-organic frameworks. Coordination Chemistry Reviews, 2011, 255, 1791-1823.	18.8	1,805
2	CO₂ Capture and Separations Using MOFs: Computational and Experimental Studies. Chemical Reviews, 2017, 117, 9674-9754.	47.7	837
3	Porous materials with pre-designed single-molecule traps for CO2 selective adsorption. Nature Communications, 2013, 4, 1538.	12.8	508
4	Kinetics and mechanism of hydrogenation of furfural on Cu/SiO2 catalysts. Journal of Catalysis, 2011, 277, 1-13.	6.2	487
5	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
6	Carbon Nanotubes and Related Nanomaterials: Critical Advances and Challenges for Synthesis toward Mainstream Commercial Applications. ACS Nano, 2018, 12, 11756-11784.	14.6	388
7	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
8	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
9	Theoretical interpretation of adsorption behavior of simple fluids in slit pores. Langmuir, 1993, 9, 1801-1814.	3.5	238
10	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
11	Lithium-Ion Batteries. , 2004, , .		233
12	Formation and Growth Mechanisms of Solid-Electrolyte Interphase Layers in Rechargeable Batteries. Chemistry of Materials, 2015, 27, 7990-8000.	6.7	225
13	Pt surface segregation in bimetallic Pt3M alloys: A density functional theory study. Surface Science, 2008, 602, 107-113.	1.9	202
14	The passivity of lithium electrodes in liquid electrolytes for secondary batteries. Nature Reviews Materials, 2021, 6, 1036-1052.	48.7	201
15	Design of Oxygen Reduction Bimetallic Catalysts:â€‰ Ab-Initio-Derived Thermodynamic Guidelines. Journal of Physical Chemistry B, 2005, 109, 18902-18906.	2.6	175
16	Structure and dynamics of graphite-supported bimetallic nanoclusters. Surface Science, 2003, 545, 163-179.	1.9	165
17	Tuning the Solid Electrolyte Interphase for Selective Liâ€and Naâ€Ion Storage in Hard Carbon. Advanced Materials, 2017, 29, 1606860.	21.0	157
18	Strategies towards enabling lithium metal in batteries: interphases and electrodes. Energy and Environmental Science, 2021, 14, 5289-5314.	30.8	156

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19	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
20	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
21	In Situ Chemical Imaging of Solid-Electrolyte Interphase Layer Evolution in Liâ€“S Batteries. Chemistry of Materials, 2017, 29, 4728-4737.	6.7	147
22	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
23	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
24	Reactivity at the Lithiumâ€“Metal Anode Surface of Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2015, 119, 26828-26839.	3.1	140
25	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
26	Water Effects on Postcombustion CO₂ Capture in Mg-MOF-74. Journal of Physical Chemistry C, 2013, 117, 3383-3388.	3.1	134
27	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
28	Building multiple adsorption sites in porous polymer networks for carbon capture applications. Energy and Environmental Science, 2013, 6, 3559.	30.8	130
29	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
30	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
31	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
32	Computational Studies of the Interactions of Oxygen with Platinum Clusters. Journal of Physical Chemistry B, 2001, 105, 9943-9952.	2.6	118
33	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
34	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
35	Melting of Bimetallic Cuâ^'Ni Nanoclusters. Journal of Physical Chemistry B, 2002, 106, 7225-7236.	2.6	107
36	Lithiumâ€Pretreated Hard Carbon as Highâ€Performance Sodiumâ€Ion Battery Anodes. Advanced Energy Materials, 2018, 8, 1801441.	19.5	105

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37	Self-Supported Hydrous Iridiumâ€“Nickel Oxide Two-Dimensional Nanoframes for High Activity Oxygen Evolution Electrocatalysts. ACS Catalysis, 2018, 8, 10498-10520.	11.2	103
38	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
39	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
40	Facet-Dependent Thermal Instability in LiCoO₂. Nano Letters, 2017, 17, 2165-2171.	9.1	99
41	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
42	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
43	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
44	Synergistic Effect of Graphene Oxide for Impeding the Dendritic Plating of Li. Advanced Functional Materials, 2018, 28, 1705917.	14.9	92
45	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
46	Associations of Alkyl Carbonates:Â Intermolecular Câ‹¯HÂ·Â·Â·O Interactions. Journal of Physical Chemistry A, 2001, 105, 9972-9982.	2.5	87
47	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
48	Long-Chain Polysulfide Retention at the Cathode of Liâ€“S Batteries. Journal of Physical Chemistry C, 2016, 120, 4296-4305.	3.1	85
49	Oxidatively stable polyaniline:polyacid electrodes for electrochemical energy storage. Physical Chemistry Chemical Physics, 2013, 15, 9654.	2.8	82
50	Properties of Small Bimetallic Niâ‹¯Cu Clusters. Journal of Physical Chemistry A, 2001, 105, 7917-7925.	2.5	81
51	Localized high concentration electrolyte behavior near a lithiumâ€“metal anode surface. Journal of Materials Chemistry A, 2019, 7, 25047-25055.	10.3	81
52	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
53	Reduction mechanisms of additives on Si anodes of Li-ion batteries. Physical Chemistry Chemical Physics, 2014, 16, 17091-17098.	2.8	80
54	Spectroelectrochemical Probing of the Strong Interaction between Platinum Nanoparticles and Graphitic Domains of Carbon. ACS Catalysis, 2013, 3, 1940-1950.	11.2	78

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55	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
56	Adsorption and Dissociation of H2O2on Pt and Ptâ”Alloy Clusters and Surfaces. Journal of Physical Chemistry B, 2006, 110, 17452-17459.	2.6	76
57	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
58	Exploring interfacial stability of solid-state electrolytes at the lithium-metal anode surface. Journal of Power Sources, 2018, 396, 782-790.	7.8	73
59	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
60	Li₂S Film Formation on Lithium Anode Surface of Liâ€“S batteries. ACS Applied Materials & Interfaces, 2016, 8, 4700-4708.	8.0	70
61	Molecular simulation of a chemical reaction in supercritical water. Journal of the American Chemical Society, 1994, 116, 2689-2690.	13.7	68
62	Density Functional Theory Study of Copper Clusters. Journal of Physical Chemistry B, 1999, 103, 2830-2840.	2.6	68
63	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
64	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
65	Nucleation of Graphene and Its Conversion to Single-Walled Carbon Nanotubes. Nano Letters, 2014, 14, 6104-6108.	9.1	67
66	Theoretical studies of the reduction of ethylene carbonate. Chemical Physics Letters, 2000, 317, 421-429.	2.6	66
67	Theoretical Studies of Proton Transfer in Water and Model Polymer Electrolyte Systems. Industrial & Engineering Chemistry Research, 2001, 40, 4789-4800.	3.7	66
68	Elucidating electrolyte decomposition under electron-rich environments at the lithium-metal anode. Physical Chemistry Chemical Physics, 2017, 19, 30861-30873.	2.8	65
69	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
70	Reversible Crosslinked Polymer Binder for Recyclable Lithium Sulfur Batteries with High Performance. Advanced Functional Materials, 2020, 30, 2003605.	14.9	63
71	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
72	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

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73	Antiâ€Oxygen Leaking LiCoO₂. Advanced Functional Materials, 2019, 29, 1901110.	14.9	60
74	Classification of adsorption behavior: simple fluids in pores of slit-shaped geometry. Fluid Phase Equilibria, 1992, 76, 21-35.	2.5	59
75	Nanotube nucleation versus carbon-catalyst adhesionâ€“Probed by molecular dynamics simulations. Journal of Chemical Physics, 2009, 131, 224501.	3.0	59
76	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
77	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
78	Revealing Charge Transport Mechanisms in Li₂S₂ for Liâ€“Sulfur Batteries. Journal of Physical Chemistry Letters, 2017, 8, 1324-1330.	4.6	56
79	Monte Carlo Simulation of Cuâ^'Ni Nanoclusters: Surface Segregation Studies. Langmuir, 2001, 17, 2047-2050.	3.5	55
80	Platinum nanoclusters on graphite substrates: a molecular dynamics study. Molecular Physics, 2002, 100, 2165-2174.	1.7	55
81	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
82	Dynamic Evolution of Supported Metal Nanocatalyst/Carbon Structure during Single-Walled Carbon Nanotube Growth. ACS Nano, 2012, 6, 720-735.	14.6	55
83	Adsorption of insoluble polysulfides Li2Sx (x = 1, 2) on Li2S surfaces. Physical Chemistry Chemical Physics, 2015, 17, 9032-9039.	2.8	53
84	First-Principles Investigation of Lithium Polysulfide Structure and Behavior in Solution. Journal of Physical Chemistry C, 2017, 121, 21105-21117.	3.1	53
85	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
86	Molecular modeling studies of polymer electrolytes for power sources. Electrochimica Acta, 2005, 50, 3788-3795.	5.2	51
87	Chemical Environment Effects on the Atomic Oxygen Absorption into Pt(111) Subsurfaces. Journal of Physical Chemistry C, 2007, 111, 17388-17396.	3.1	50
88	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
89	Ion Solvation in Supercritical Water Based on an Adsorption Analogy. Journal of Physical Chemistry B, 1997, 101, 7998-8005.	2.6	48
90	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

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91	Surface segregation in bimetallic Pt3M (M=Fe, Co, Ni) alloys with adsorbed oxygen. Surface Science, 2009, 603, 349-353.	1.9	46
92	Molecular dynamics studies of a model polymerâ€“catalystâ€“carbon interface. Electrochimica Acta, 2006, 51, 5904-5911.	5.2	45
93	Theoretical analysis of reactivity on Pt(111) and Ptâ€“Pd(111) alloys. Surface Science, 2007, 601, 4786-4792.	1.9	45
94	Size effect on the stability of Cuâ€“Ag nanoalloys. Molecular Simulation, 2009, 35, 785-794.	2.0	45
95	Oxygen reduction on a platinum cluster. Chemical Physics Letters, 2003, 367, 439-447.	2.6	44
96	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
97	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
98	Surface segregation of core atoms in coreâ€“shell structures. Chemical Physics Letters, 2008, 456, 64-67.	2.6	43
99	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
100	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
101	Isosteric Heats of Adsorption on Carbon Predicted by Density Functional Theory. Industrial & Engineering Chemistry Research, 1998, 37, 1159-1166.	3.7	42
102	Geometric and Electronic Confinement Effects on Catalysis. Journal of Physical Chemistry C, 2011, 115, 21324-21333.	3.1	42
103	Direct evidence of atomic-scale structural fluctuations in catalyst nanoparticles. Journal of Catalysis, 2017, 349, 149-155.	6.2	41
104	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
105	Effects of charged interfaces on electrolyte decomposition at the lithium metal anode. Journal of Power Sources, 2020, 472, 228449.	7.8	41
106	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
107	Molecular dynamics simulations of metal-organic frameworks as membranes for gas mixtures separation. Journal of Membrane Science, 2013, 428, 241-250.	8.2	40
108	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

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109	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
110	Phase Behavior of Methaneâ€“Ethane Mixtures in Nanopores. Industrial & Engineering Chemistry Research, 2017, 56, 11634-11643.	3.7	39
111	A Latticeâ€Gas Model Study of Lithium Intercalation in Graphite. Journal of the Electrochemical Society, 1999, 146, 3630-3638.	2.9	38
112	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
113	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
114	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
115	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
116	Molecular dynamics studies of phonon spectra in mono- and bimetallic nanoclusters. Surface Science, 2005, 581, 213-224.	1.9	37
117	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
118	Role of the Catalyst in the Growth of Single-Wall Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2006, 6, 1247-1258.	0.9	37
119	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
120	The role of cap chirality in the mechanism of growth of single-wall carbon nanotubes. Nanotechnology, 2008, 19, 485604.	2.6	37
121	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
122	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
123	Molecular Dynamics Study of Graphite/Electrolyte Interfaces. Journal of the Electrochemical Society, 2001, 148, A624.	2.9	36
124	Nanocatalyst structure as a template to define chirality of nascent single-walled carbon nanotubes. Journal of Chemical Physics, 2011, 134, 014705.	3.0	36
125	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
126	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

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127	Dealloying of platinum-based alloy catalysts: Kinetic Monte Carlo simulations. Electrochimica Acta, 2013, 101, 326-333.	5.2	35
128	Surface segregation in bimetallic nanoclusters: Geometric and thermodynamic effects. International Journal of Quantum Chemistry, 2001, 85, 580-591.	2.0	34
129	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
130	Atomic Oxygen Absorption into Pt-Based Alloy Subsurfaces. Journal of Physical Chemistry C, 2008, 112, 5057-5065.	3.1	34
131	Ethanol Reforming on Co(0001) Surfaces: A Density Functional Theory Study. Journal of Physical Chemistry A, 2012, 116, 1409-1416.	2.5	34
132	Classical Molecular Dynamics of Clathrateâˆ'Methaneâˆ'Waterâˆ'Kinetic Inhibitor Composite Systemsâ€. Journal of Physical Chemistry C, 2007, 111, 15554-15564.	3.1	33
133	Density functional theory analysis of reactivity of PtxPdy alloy clusters. Surface Science, 2007, 601, 165-171.	1.9	32
134	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
135	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
136	Chemical and mechanical degradation and mitigation strategies for Si anodes. Journal of Power Sources, 2019, 419, 208-218.	7.8	32
137	Mesoscale Anatomy of Dead Lithium Formation. Journal of Physical Chemistry C, 2020, 124, 6502-6511.	3.1	31
138	Hydrogen and Oxygen Adsorption on Rhn (n = 1âˆ'6) Clusters. Journal of Physical Chemistry A, 2003, 107, 10370-10380.	2.5	30
139	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
140	Lithium oxidation and electrolyte decomposition at Li-metal/liquid electrolyte interfaces. Journal of Materials Chemistry A, 2020, 8, 17036-17055.	10.3	28
141	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
142	Vibrational Spectra of Anhydrous and Monohydrated Caffeine and Theophylline Molecules and Crystals. Journal of Physical Chemistry A, 2008, 112, 10210-10219.	2.5	27
143	Electrolyte materials - Issues and challenges. AIP Conference Proceedings, 2014, , .	0.4	27
144	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

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145	Exploring the LiOH Formation Reaction Mechanism in Lithiumâ€“Air Batteries. Chemistry of Materials, 2018, 30, 708-717.	6.7	27
146	Catalytic Upgrading of Methane to Higher Hydrocarbon in a Nonoxidative Chemical Conversion. Energy & Fuels, 2016, 30, 2584-2593.	5.1	26
147	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
148	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
149	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
150	Designing oxygen reduction catalysts: Insights from metalloenzymes. Chemical Physics Letters, 2007, 440, 130-133.	2.6	23
151	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
152	Characterization of carbon atomistic pathways during single-walled carbon nanotube growth on supported metal nanoparticles. Carbon, 2013, 57, 298-309.	10.3	23
153	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
154	Molecular dynamics simulations of cinchonidine-modified platinum in ethanol: comparisons with surface studies. Surface Science, 2004, 563, 57-73.	1.9	22
155	Effects of water and electric field on atomic oxygen adsorption on Ptâ€“Co alloys. Surface Science, 2009, 603, 3239-3248.	1.9	22
156	Open Framework Allotropes of Silicon: Potential Anode Materials for Na and Li-ion Batteries. Electrochimica Acta, 2016, 207, 301-307.	5.2	22
157	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
158	Computational Study of the Evolution of Ni-Based Catalysts during the Dry Reforming of Methane. Energy & Fuels, 2020, 34, 4855-4864.	5.1	22
159	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
160	Surface atomic distribution and water adsorption on Ptâ€“Co alloys. Surface Science, 2009, 603, 912-920.	1.9	20
161	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
162	Hydrogen evolution reaction mechanism on Ti₃C₂ MXene revealed by in situ/operando Raman spectroelectrochemistry. Nanoscale, 2022, 14, 5068-5078.	5.6	20

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163	Effect of Nanotube Length on the Aromaticity of Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2008, 112, 3482-3488.	3.1	19
164	Growth of Carbon Structures on Stepped (211)Co Surfaces. Journal of Physical Chemistry C, 2009, 113, 15658-15666.	3.1	19
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