Angelos Michaelides

List of Publications by Year
in descending order

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		9234	6630
211	25,520	74	156
papers	citations	h-index	g-index

218	218	218	22365
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Van der Waals density functionals applied to solids. Physical Review B, 2011, 83, .	1.1	3,608
2	Chemical accuracy for the van der Waals density functional. Journal of Physics Condensed Matter, 2010, 22, 022201.	0.7	2,222
3	Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory. Journal of Chemical Physics, 2012, 137, 120901.	1.2	931
4	Crystal Nucleation in Liquids: Open Questions and Future Challenges in Molecular Dynamics Simulations. Chemical Reviews, 2016, 116, 7078-7116.	23.0	635
5	Perspective: How good is DFT for water?. Journal of Chemical Physics, 2016, 144, 130901.	1.2	571
6	A molecular perspective of water at metal interfaces. Nature Materials, 2012, 11, 667-674.	13.3	568
7	Identification of General Linear Relationships between Activation Energies and Enthalpy Changes for Dissociation Reactions at Surfaces. Journal of the American Chemical Society, 2003, 125, 3704-3705.	6.6	536
8	Water at Interfaces. Chemical Reviews, 2016, 116, 7698-7726.	23.0	536
9	Pt/Cu single-atom alloys as coke-resistant catalysts for efficient Câ€“H activation. Nature Chemistry, 2018, 10, 325-332.	6.6	472
10	Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges. Chemical Reviews, 2016, 116, 7529-7550.	23.0	439
11	Stone-Wales defects in graphene and other planar<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>2</mml:mn></mml:msup></mml:m materials. Physical Review B, 2009, 80, .	1.1	422
12	Quantum nature of the hydrogen bond. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6369-6373.	3.3	360
13	General Model for Water Monomer Adsorption on Close-Packed Transition and Noble Metal Surfaces. Physical Review Letters, 2003, 90, 216102.	2.9	358
14	Friction of Water on Graphene and Hexagonal Boron Nitride from Ab Initio Methods: Very Different Slippage Despite Very Similar Interface Structures. Nano Letters, 2014, 14, 6872-6877.	4.5	326
15	Catalytic Water Formation on Platinum:â€‰ A First-Principles Study. Journal of the American Chemical Society, 2001, 123, 4235-4242.	6.6	314
16	Ice nanoclusters at hydrophobic metalÂsurfaces. Nature Materials, 2007, 6, 597-601.	13.3	303
17	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. Physical Review B, 2012, 86, .	1.1	243
18	Atomistic details of oxide surfaces and surface oxidation: the example of copper and its oxides. Surface Science Reports, 2015, 70, 424-447.	3.8	237

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19	Structure of a model TiO2Âphotocatalytic interface. Nature Materials, 2017, 16, 461-466.	13.3	234
20	Active sites in heterogeneous ice nucleationâ€"the example of K-rich feldspars. Science, 2017, 355, 367-371.	6.0	231
21	Different Surface Chemistries of Water on Ru{0001}:Â From Monomer Adsorption to Partially Dissociated Bilayers. Journal of the American Chemical Society, 2003, 125, 2746-2755.	6.6	228
22	Adsorption and diffusion of water on graphene from first principles. Physical Review B, 2011, 84, .	1.1	218
23	A one-dimensional ice structure built from pentagons. Nature Materials, 2009, 8, 427-431.	13.3	212
24	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters. II. The water hexamer and van der Waals interactions. Journal of Chemical Physics, 2008, 129, 194111.	1.2	211
25	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters: Benchmarks approaching the complete basis set limit. Journal of Chemical Physics, 2007, 127, 184104.	1.2	208
26	Lonely Atoms with Special Gifts: Breaking Linear Scaling Relationships in Heterogeneous Catalysis with Single-Atom Alloys. Journal of Physical Chemistry Letters, 2018, 9, 5636-5646.	2.1	206
27	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	2.9	193
28	First-principles design of a single-atomâ€"alloy propane dehydrogenation catalyst. Science, 2021, 372, 1444-1447.	6.0	185
29	Structure and dynamics of liquid water on rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2010, 82, .	1.1	182
30	The Many Faces of Heterogeneous Ice Nucleation: Interplay Between Surface Morphology and Hydrophobicity. Journal of the American Chemical Society, 2015, 137, 13658-13669.	6.6	182
31	A density functional theory study of hydroxyl and the intermediate in the water formation reaction on Pt. Journal of Chemical Physics, 2001, 114, 513.	1.2	173
32	Novel Water Overlayer Growth on Pd(111) Characterized with Scanning Tunneling Microscopy and Density Functional Theory. Physical Review Letters, 2004, 93, 116101.	2.9	173
33	The role of van der Waals forces in water adsorption on metals. Journal of Chemical Physics, 2013, 138, 024708.	1.2	173
34	Controlling Hydrogen Activation, Spillover, and Desorption with Pdâ€"Au Single-Atom Alloys. Journal of Physical Chemistry Letters, 2016, 7, 480-485.	2.1	169
35	Two Dimensional Ice from First Principles: Structures and Phase Transitions. Physical Review Letters, 2016, 116, 025501.	2.9	167
36	Insight intoH2O-ice adsorption and dissociation on metal surfaces from first-principles simulations. Physical Review B, 2004, 69, .	1.1	161

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37	To Wet or Not to Wet? Dispersion Forces Tip the Balance for Water Ice on Metals. Physical Review Letters, 2011, 106, 026101.	2.9	159
38	Insight into the description of van der Waals forces for benzene adsorption on transition metal (111) surfaces. Journal of Chemical Physics, 2014, 140, 084704.	1.2	158
39	Fast diffusion of water nanodroplets on graphene. Nature Materials, 2016, 15, 66-71.	13.3	156
40	Water on the hydroxylated (001) surface of kaolinite: From monomer adsorption to a flat 2D wetting layer. Surface Science, 2008, 602, 960-974.	0.8	155
41	Elucidating the Stability and Reactivity of Surface Intermediates on Single-Atom Alloy Catalysts. ACS Catalysis, 2018, 8, 5038-5050.	5.5	152
42	Density functional theory simulations of waterâ€“metal interfaces: waltzing waters, a novel 2D ice phase, and more. Applied Physics A: Materials Science and Processing, 2006, 85, 415-425.	1.1	150
43	Improved description of soft layered materials with van der Waals density functional theory. Journal of Physics Condensed Matter, 2012, 24, 424216.	0.7	150
44	Insight into Microscopic Reaction Pathways in Heterogeneous Catalysis. Journal of the American Chemical Society, 2000, 122, 9866-9867.	6.6	146
45	Revisiting the Structure of thep(4Ã—4)Surface Oxide on Ag(111). Physical Review Letters, 2006, 96, 146101.	2.9	144
46	Development of a machine learning potential for graphene. Physical Review B, 2018, 97, .	1.1	142
47	Surface premelting of water ice. Nature Reviews Chemistry, 2019, 3, 172-188.	13.8	142
48	An accurate and transferable machine learning potential for carbon. Journal of Chemical Physics, 2020, 153, 034702.	1.2	137
49	Resolution of an Ancient Surface Science Anomaly: Work Function Change Induced by N Adsorption onW{100}. Physical Review Letters, 2003, 90, 246103.	2.9	122
50	Molecular simulations of heterogeneous ice nucleation. I. Controlling ice nucleation through surface hydrophilicity. Journal of Chemical Physics, 2015, 142, 184704.	1.2	122
51	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. Journal of Chemical Physics, 2013, 139, 154702.	1.2	119
52	Carbon Monoxide Poisoning Resistance and Structural Stability of Single Atom Alloys. Topics in Catalysis, 2018, 61, 428-438.	1.3	117
53	Water Dimer Diffusion on Pd{111} Assisted by an H-Bond Donor-Acceptor Tunneling Exchange. Physical Review Letters, 2004, 92, 136104.	2.9	114
54	Structures and thermodynamic phase transitions for oxygen and silver oxide phases on Ag{1 1 1}. Chemical Physics Letters, 2003, 367, 344-350.	1.2	113

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55	Positive Charge States and Possible Polymorphism of Gold Nanoclusters on Reduced Ceria. Journal of the American Chemical Society, 2010, 132, 2175-2182.	6.6	109
56	New Insights into Ethene Epoxidation on Two Oxidized Ag{111} Surfaces. Journal of the American Chemical Society, 2003, 125, 5620-5621.	6.6	108
57	When seeing is not believing: Oxygen on Ag(111), a simple adsorption system?. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2005, 23, 1487-1497.	0.9	108
58	Theory of gold on ceria. Physical Chemistry Chemical Physics, 2011, 13, 22-33.	1.3	108
59	Structure of gold atoms on stoichiometric and defective ceria surfaces. Journal of Chemical Physics, 2008, 129, 194708.	1.2	103
60	Oxygen vacancy clusters on ceria: Decisive role of cerium<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>f</mml:mi></mml:math>electrons. Physical Review B, 2009, 79, .	1.1	103
61	Ice formation on kaolinite: Lattice match or amphoterism?. Surface Science, 2007, 601, 5378-5381.	0.8	101
62	Quantum Nature of the Proton in Water-Hydroxyl Overlayers on Metal Surfaces. Physical Review Letters, 2010, 104, 066102.	2.9	101
63	Physical origin of the high reactivity of subsurface hydrogen in catalytic hydrogenation. Journal of Chemical Physics, 1999, 111, 1343-1345.	1.2	94
64	Insight from first principles into the nature of the bonding between water molecules and 4d metal surfaces. Journal of Chemical Physics, 2009, 130, 184707.	1.2	94
65	Experimental and theoretical study of oxygen adsorption structures on Ag(111). Physical Review B, 2009, 80, .	1.1	90
66	Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods. Journal of Physical Chemistry Letters, 2019, 10, 358-368.	2.1	90
67	Cation-controlled wetting properties of vermiculite membranes and its promise for fouling resistant oilâ€“water separation. Nature Communications, 2020, 11, 1097.	5.8	89
68	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>c</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>2</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>2</mml:mn><mml:mo) TjET Qq0 0 0 rgBT /Ov by Bjerrum Defects. Physical Review Letters, 2011, 106, 046103.	2.9	85
69	Methyl chemisorption on Ni(111) and C H M multicentre bonding: a density functional theory study. Surface Science, 1999, 437, 362-376.	0.8	84
70	Solvent-Induced Proton Hopping at a Waterâ€“Oxide Interface. Journal of Physical Chemistry Letters, 2014, 5, 474-480.	2.1	82
71	Machine learning potentials for complex aqueous systems made simple. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	82
72	The microscopic features of heterogeneous ice nucleation may affect the macroscopic morphology of atmospheric ice crystals. Faraday Discussions, 2013, 167, 389.	1.6	80

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73	Anchoring Sites for Initial Au Nucleation on CeO₂{111}: O Vacancy versus Ce Vacancy. Journal of Physical Chemistry C, 2009, 113, 6411-6417.	1.5	79
74	Ice is born in low-mobility regions of supercooled liquid water. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 2009-2014.	3.3	79
75	Microscopic Mechanism and Kinetics of Ice Formation at Complex Interfaces: Zooming in on Kaolinite. Journal of Physical Chemistry Letters, 2016, 7, 2350-2355.	2.1	77
76	Quantum simulation of low-temperature metallic liquid hydrogen. Nature Communications, 2013, 4, 2064.	5.8	75
77	The water-benzene interaction: Insight from electronic structure theories. Journal of Chemical Physics, 2009, 130, 154303.	1.2	73
78	Formation of Methane Hydrate in the Presence of Natural and Synthetic Nanoparticles. Journal of the American Chemical Society, 2018, 140, 3277-3284.	6.6	73
79	Molecular simulations of heterogeneous ice nucleation. II. Peeling back the layers. Journal of Chemical Physics, 2015, 142, 184705.	1.2	72
80	The Carbon-Water Interface: Modeling Challenges and Opportunities for the Water-Energy Nexus. Annual Review of Chemical and Biomolecular Engineering, 2016, 7, 533-556.	3.3	72
81	Surface Energy and Surface Proton Order of Ice<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="normal">I</mml:mi><mml:mi>h</mml:mi></mml:math>. Physical Review Letters, 2008, 101, 155703.	2.9	70
82	Influence of water on the electronic structure of metal-supported graphene: Insights from van der Waals density functional theory. Physical Review B, 2012, 85, .	1.1	70
83	Preparation, Structure, and Surface Chemistry of Niâ€“Au Single Atom Alloys. Journal of Physical Chemistry C, 2016, 120, 13574-13580.	1.5	70
84	Encapsulation and Polymerization of White Phosphorus Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie - International Edition, 2017, 56, 8144-8148.	7.2	70
85	Fast and accurate quantum Monte Carlo for molecular crystals. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 1724-1729.	3.3	69
86	Melting the Ice: On the Relation between Melting Temperature and Size for Nanoscale Ice Crystals. ACS Nano, 2011, 5, 4562-4569.	7.3	65
87	Manipulation and Control of Hydrogen Bond Dynamics in Absorbed Ice Nanoclusters. Physical Review Letters, 2008, 101, 136102.	2.9	64
88	Coupled cluster benchmarks of water monomers and dimers extracted from density-functional theory liquid water: The importance of monomer deformations. Journal of Chemical Physics, 2009, 131, 124509.	1.2	62
89	Softened Câ€“H modes of adsorbed methyl and their implications for dehydrogenation: An ab initio study. Journal of Chemical Physics, 2001, 114, 2523-2526.	1.2	61
90	Proton ordering in cubic ice and hexagonal ice; a potential new ice phaseâ€”XIc. Physical Chemistry Chemical Physics, 2011, 13, 19788.	1.3	60

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91	Understanding corrosion inhibition with van der Waals DFT methods: the case of benzotriazole. Faraday Discussions, 2015, 180, 439-458.	1.6	60
92	Large variation of vacancy formation energies in the surface of crystalline ice. Nature Materials, 2011, 10, 794-798.	13.3	59
93	Quantum Effects in the Diffusion of Hydrogen on Ru(0001). Journal of Physical Chemistry Letters, 2013, 4, 1565-1569.	2.1	59
94	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. Journal of Chemical Physics, 2015, 142, 181101.	1.2	56
95	Pre-critical fluctuations and what they disclose about heterogeneous crystal nucleation. Nature Communications, 2017, 8, 2257.	5.8	55
96	A critical assessment of theoretical methods for finding reaction pathways and transition states of surface processes. Journal of Physics Condensed Matter, 2010, 22, 074203.	0.7	54
97	Boosting the accuracy and speed of quantum Monte Carlo: Size consistency and time step. Physical Review B, 2016, 93, .	1.1	54
98	A first principles study of CH3 dehydrogenation on Ni(111). Journal of Chemical Physics, 2000, 112, 8120-8125.	1.2	53
99	Density functional theory study of the interaction of monomeric water with the Ag{111} surface. Physical Review B, 2004, 69, .	1.1	53
100	Non-hexagonal ice at hexagonal surfaces: the role of lattice mismatch. Physical Chemistry Chemical Physics, 2012, 14, 7944.	1.3	53
101	Ice formation on kaolinite: Insights from molecular dynamics simulations. Journal of Chemical Physics, 2016, 145, 211927.	1.2	53
102	A density functional theory study of CH2 and H adsorption on Ni(111). Journal of Chemical Physics, 2000, 112, 6006-6014.	1.2	52
103	Initial stages of salt crystal dissolution determined with ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2011, 13, 13162.	1.3	51
104	Nature of proton transport in a water-filled carbon nanotube and in liquid water. Physical Chemistry Chemical Physics, 2013, 15, 6344.	1.3	51
105	Hydrogenation Facilitates Proton Transfer through Two-Dimensional Honeycomb Crystals. Journal of Physical Chemistry Letters, 2017, 8, 6009-6014.	2.1	51
106	Binding of hydrogen on benzene, coronene, and graphene from quantum Monte Carlo calculations. Journal of Chemical Physics, 2011, 134, 134701.	1.2	48
107	Interaction between water and carbon nanostructures: How good are current density functional approximations?. Journal of Chemical Physics, 2019, 151, 164702.	1.2	47
108	Hydrogenation of S to H2S on Pt(111): A first-principles study. Journal of Chemical Physics, 2001, 115, 8570-8574.	1.2	46

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109	Evidence for stable square ice from quantum Monte Carlo. Physical Review B, 2016, 94, .	1.1	46
110	Inverse Temperature Dependence of Nuclear Quantum Effects in DNA Base Pairs. Journal of Physical Chemistry Letters, 2016, 7, 2125-2131.	2.1	46
111	Simultaneous Deep Tunneling and Classical Hopping for Hydrogen Diffusion on Metals. Physical Review Letters, 2017, 119, 126001.	2.9	46
112	Interfacial water: A first principles molecular dynamics study of a nanoscale water film on salt. Journal of Chemical Physics, 2009, 130, 234702.	1.2	45
113	The Energy of Hydroxyl Coadsorbed with Water on Pt(111). Journal of Physical Chemistry C, 2011, 115, 23008-23012.	1.5	45
114	Water-hydroxyl phases on an open metal surface: breaking the ice rules. Chemical Science, 2012, 3, 93-102.	3.7	45
115	Significant Quantum Effects in Hydrogen Activation. ACS Nano, 2014, 8, 4827-4835.	7.3	44
116	Stability of Complex Biomolecular Structures: van der Waals, Hydrogen Bond Cooperativity, and Nuclear Quantum Effects. Journal of Physical Chemistry Letters, 2015, 6, 4233-4238.	2.1	43
117	Can Ice-Like Structures Form on Non-Ice-Like Substrates? The Example of the K-feldspar Microcline. Journal of Physical Chemistry C, 2016, 120, 6704-6713.	1.5	43
118	What makes a good descriptor for heterogeneous ice nucleation on OH-patterned surfaces. Physical Review B, 2017, 96, .	1.1	43
119	Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. Journal of Chemical Physics, 2017, 147, 044710.	1.2	43
120	Unravelling the origins of ice nucleation on organic crystals. Chemical Science, 2018, 9, 8077-8088.	3.7	43
121	Simulating ice nucleation, one molecule at a time, with the â€˜DFT microscopeâ€™. Faraday Discussions, 2007, 136, 287.	1.6	42
122	Visualization of Hydrogen Bonding and Associated Chirality in Methanol Hexamers. Physical Review Letters, 2011, 107, 256101.	2.9	42
123	Cooperative Interplay of van der Waals Forces and Quantum Nuclear Effects on Adsorption: H at Graphene and at Coronene. ACS Nano, 2014, 8, 9905-9913.	7.3	42
124	Density Oscillations in a Nanoscale Water Film on Salt: Insight from Ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2008, 130, 8572-8573.	6.6	41
125	Benchmarking the performance of density functional theory and point charge force fields in their description of sI methane hydrate against diffusion Monte Carlo. Journal of Chemical Physics, 2014, 140, 174703.	1.2	41
126	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M₂(dobdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry A, 2017, 121, 4139-4151.	1.1	41

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127	Density functional theory study of flat and stepped NaCl(001). Physical Review B, 2007, 76, .	1.1	40
128	On thin ice: surface order and disorder during pre-melting. Faraday Discussions, 2009, 141, 277-292.	1.6	40
129	Surface energy and surface proton order of the ice Ih basal and prism surfaces. Journal of Physics Condensed Matter, 2010, 22, 074209.	0.7	40
130	Trends in water monomer adsorption and dissociation on flat insulating surfaces. Physical Chemistry Chemical Physics, 2011, 13, 12447.	1.3	40
131	Understanding the role of ions and water molecules in the NaCl dissolution process. Journal of Chemical Physics, 2013, 139, 234702.	1.2	40
132	First-principles study ofH2Odiffusion on a metal surface:â€ƒH2Oon Al{100}. Physical Review B, 2004, 69, .	1.1	39
133	Origins of fast diffusion of water dimers on surfaces. Nature Communications, 2020, 11, 1689.	5.8	39
134	How strongly do hydrogen and water molecules stick to carbon nanomaterials?. Journal of Chemical Physics, 2017, 146, .	1.2	38
135	Is High-Density Amorphous Ice Simply a â€œDerailedâ€•State along the Ice I to Ice IV Pathway?. Journal of Physical Chemistry Letters, 2017, 8, 1645-1650.	2.1	38
136	Local Investigation of Femtosecond Laser Induced Dynamics of Water Nanoclusters on Cu(111). Physical Review Letters, 2009, 103, 026101.	2.9	37
137	A density functional theory study of the reaction of C+O, C+N, and C+H on close packed metal surfaces. Journal of Chemical Physics, 2001, 114, 5792-5795.	1.2	35
138	A comparison between quantum chemistry and quantum Monte Carlo techniques for the adsorption of water on the (001) LiH surface. Journal of Chemical Physics, 2017, 146, 204108.	1.2	35
139	Predicting heterogeneous ice nucleation with a data-driven approach. Nature Communications, 2020, 11, 4777.	5.8	35
140	Electronic structure software. Journal of Chemical Physics, 2020, 153, 070401.	1.2	34
141	Strong Coupling between Nanofluidic Transport and Interfacial Chemistry: How Defect Reactivity Controls Liquidâ€“Solid Friction through Hydrogen Bonding. Journal of Physical Chemistry Letters, 2016, 7, 1381-1386.	2.1	33
142	Acetone adsorption on ice investigated by X-ray spectroscopy and density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 19988.	1.3	32
143	Waterâ€“Ice Analogues of Polycyclic Aromatic Hydrocarbons: Water Nanoclusters on Cu(111). Journal of the American Chemical Society, 2017, 139, 6403-6410.	6.6	32
144	The kaolinite (001) polar basal plane. Surface Science, 2010, 604, 111-117.	0.8	30

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145	Reply to â€œComment on `Structure and dynamics of liquid water on rutile TiO2(110)'â€‰â€• Physical Review B, 2012, 85, .	1.1	30
146	Enhancement of low-energy electron emission in 2D radioactive films. Nature Materials, 2015, 14, 904-907.	13.3	30
147	Toward Accurate Adsorption Energetics on Clay Surfaces. Journal of Physical Chemistry C, 2016, 120, 26402-26413.	1.5	30
148	Double-layer ice from first principles. Physical Review B, 2017, 95, .	1.1	29
149	Defect-Dependent Corrugation in Graphene. Nano Letters, 2021, 21, 8143-8150.	4.5	29
150	Proton transfer in adsorbed water dimers. Physical Chemistry Chemical Physics, 2010, 12, 3953.	1.3	28
151	Hydrogen-bonded assembly of methanol on Cu(111). Physical Chemistry Chemical Physics, 2012, 14, 11846.	1.3	28
152	Visualization of Water-Induced Surface Segregation of Polarons on Rutile TiO₂(110). Journal of Physical Chemistry Letters, 2018, 9, 4865-4871.	2.1	28
153	Direct assessment of quantum nuclear effects on hydrogen bond strength by constrained-centroid ab initio path integral molecular dynamics. Journal of Chemical Physics, 2010, 133, 174306.	1.2	26
154	Structure and energetics of hydrogen-bonded networks of methanol on close packed transition metal surfaces. Journal of Chemical Physics, 2014, 141, 014701.	1.2	26
155	Encapsulation and Polymerization of White Phosphorus Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie, 2017, 129, 8256-8260.	1.6	26
156	Classical and quantum ordering of protons in cold solid hydrogen under megabar pressures. Journal of Physics Condensed Matter, 2013, 25, 085402.	0.7	25
157	Water on BN doped benzene: A hard test for exchange-correlation functionals and the impact of exact exchange on weak binding. Journal of Chemical Physics, 2014, 141, 18C530.	1.2	25
158	Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives. Journal of Chemical Physics, 2017, 147, 164113.	1.2	25
159	A new scheme for fixed node diffusion quantum Monte Carlo with pseudopotentials: Improving reproducibility and reducing the trial-wave-function bias. Journal of Chemical Physics, 2019, 151, 134105.	1.2	25
160	Machine Learning Potential for Hexagonal Boron Nitride Applied to Thermally and Mechanically Induced Rippling. Journal of Physical Chemistry C, 2020, 124, 22278-22290.	1.5	25
161	Water Flow in Single-Wall Nanotubes: Oxygen Makes It Slip, Hydrogen Makes It Stick. ACS Nano, 2022, 16, 10775-10782.	7.3	25
162	Slippery when narrow. Nature, 2016, 537, 171-172.	13.7	24

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163	Strain Relief during Ice Growth on a Hexagonal Template. Journal of the American Chemical Society, 2019, 141, 8599-8607.	6.6	24
164	Oneâ€Dimensional Arsenic Allotropes: Polymerization of Yellow Arsenic Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie - International Edition, 2018, 57, 11649-11653.	7.2	23
165	Adsorption Behavior of Organic Molecules: A Study of Benzotriazole on Cu(111) with Spectroscopic and Theoretical Methods. Langmuir, 2019, 35, 882-893.	1.6	22
166	Microscopic Kinetics Pathway of Salt Crystallization in Graphene Nanocapillaries. Physical Review Letters, 2021, 126, 136001.	2.9	22
167	How strong is the bond between water and salt?. Surface Science, 2008, 602, L135-L138.	0.8	21
168	Tuning dissociation using isoelectronically doped graphene and hexagonal boron nitride: Water and other small molecules. Journal of Chemical Physics, 2016, 144, 154706.	1.2	20
169	Heterogeneous seeded molecular dynamics as a tool to probe the ice nucleating ability of crystalline surfaces. Journal of Chemical Physics, 2018, 149, 072327.	1.2	20
170	Anomalously Low Barrier for Water Dimer Diffusion on Cu(111). Nano Letters, 2019, 19, 3049-3056.	4.5	20
171	Communication: Ab initio simulations of hydrogen-bonded ferroelectrics: Collective tunneling and the origin of geometrical isotope effects. Journal of Chemical Physics, 2014, 140, 041103.	1.2	19
172	The interplay of covalency, hydrogen bonding, and dispersion leads to a long range chiral network: The example of 2-butanol. Journal of Chemical Physics, 2016, 144, 094703.	1.2	19
173	Carbon Monoxide Mediated Hydrogen Release from PtCu Single-Atom Alloys: The Punctured Molecular Cork Effect. Journal of Physical Chemistry C, 2019, 123, 10419-10428.	1.5	19
174	Melting the ice one layer at a time. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 195-197.	3.3	18
175	One-Dimensional Pnictogen Allotropes inside Single-Wall Carbon Nanotubes. Inorganic Chemistry, 2019, 58, 15216-15224.	1.9	18
176	The quantum nature of hydrogen. International Reviews in Physical Chemistry, 2019, 38, 35-61.	0.9	18
177	Initial stages in the oxidation and reduction of the4Ã—4surface oxide phase on Ag{111}: A combined density-functional theory and STM simulation study. Physical Review B, 2003, 68, .	1.1	17
178	Hydration of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msubsup><mml:mrow><mml:mi>NH</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn><mml:mo> in Water: Bifurcated Hydrogen Bonding Structures and Fast Rotational Dynamics. Physical Review Letters, 2020, 125, 106001.	2.9	17
179	Water/oil interfacial tension reduction â€“ an interfacial entropy driven process. Physical Chemistry Chemical Physics, 2021, 23, 25075-25085.	1.3	17
180	Understanding the interaction of organic corrosion inhibitors with copper at the molecular scale: Benzotriazole on Cu(110). Applied Surface Science, 2021, 570, 151206.	3.1	16

#	Article	IF	Citations
181	Periodic Trends in Adsorption Energies around Single-Atom Alloy Active Sites. Journal of Physical Chemistry Letters, 2021, 12, 10060-10067.	2.1	16
182	Small polarons and the Janus nature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml (110). Physical Review B, 2020, 101, .	1.1	15
183	Routes to cubic ice through heterogeneous nucleation. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	15
184	Dynamics of quantum tunneling: Effects on the rate and transition path of OH on Cu(110). Physical Review B, 2010, 81, .	1.1	14
185	A Blue-Sky Approach to Understanding Cloud Formation. Bulletin of the American Meteorological Society, 2016, 97, 1797-1802.	1.7	14
186	Quantum nuclear effects on the location of hydrogen above and below the palladium (100) surface. Surface Science, 2011, 605, 689-694.	0.8	13
187	Communication: Truncated non-bonded potentials can yield unphysical behavior in molecular dynamics simulations of interfaces. Journal of Chemical Physics, 2017, 147, 121102.	1.2	13
188	The color center singlet state of oxygen vacancies in TiO2. Journal of Chemical Physics, 2020, 153, 204704.	1.2	13
189	Corrosion control: general discussion. Faraday Discussions, 2015, 180, 543-576.	1.6	12
190	â€œTextbookâ€•Adsorption at â€œNontextbookâ€•Adsorption Sites: Halogen Atoms on Alkali Halide Surfaces. Physical Review Letters, 2006, 97, 046802.	2.9	10
191	Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. Journal of Chemical Physics, 2015, 143, 102601.	1.2	10
192	The role of structural order in heterogeneous ice nucleation. Chemical Science, 2022, 13, 5014-5026.	3.7	10
193	Chirality at two-dimensional surfaces: A perspective from small molecule alcohol assembly on Au(111). Journal of Chemical Physics, 2018, 149, 034703.	1.2	9
194	General embedded cluster protocol for accurate modeling of oxygen vacancies in metal-oxides. Journal of Chemical Physics, 2022, 156, 124704.	1.2	9
195	Long-Range Ionic and Short-Range Hydration Effects Govern Strongly Anisotropic Clay Nanoparticle Interactions. Journal of Physical Chemistry C, 2022, 126, 8143-8151.	1.5	7
196	The unhappy marriage of transition and noble metal atoms: A new way to enhance catalytic activity? (A) Tj ETQq0 0 0 rgBT /Overlock 10 2007, 601, 3529-3531.	0.8	6
197	Atomic-Scale Picture of the Composition, Decay, and Oxidation of Two-Dimensional Radioactive Films. ACS Nano, 2016, 10, 2152-2158.	7.3	5
198	Rapid Water Diffusion at Cryogenic Temperatures through an Inchworm-like Mechanism. Nano Letters, 2022, 22, 340-346.	4.5	5

#	Article	IF	Citations
199	The Valency Effect on Reaction Pathways in Heterogeneous Catalysis: Insight from Density Functional Theory Calculations. Progress in Theoretical Chemistry and Physics, 2001, , 199-215.	0.2	4
200	How do interfaces alter the dynamics of supercooled water?. Nanoscale, 2022, 14, 4254-4262.	2.8	4
201	EXPLORING THE CATALYTIC ACTIVITY OF A NOBLE METAL: THE Ag CATALYZED ETHYLENE EPOXIDATION REACTION. , 2006, , 389-424.		3
202	Can molecular simulations reliably compare homogeneous and heterogeneous ice nucleation?. Journal of Chemical Physics, 2022, 156, 164501.	1.2	3
203	Sticky when wet. Nature Chemistry, 2018, 10, 376-377.	6.6	2
204	Oneâ€Dimensional Arsenic Allotropes: Polymerization of Yellow Arsenic Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie, 2018, 130, 11823-11827.	1.6	2
205	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	1.2	2
206	Chemical physics software. Journal of Chemical Physics, 2021, 155, 010401.	1.2	2
207	Interplay of structural and dynamical heterogeneity in the nucleation mechanism in nickel. Faraday Discussions, 2022, 235, 406-415.	1.6	2
208	Observation and Characterization of Dicarbonyls on a RhCu Single-Atom Alloy. Journal of Physical Chemistry Letters, 2022, 13, 6316-6322.	2.1	2
209	Editorial: The Future of Chemical Physics Conference 2016. Journal of Chemical Physics, 2016, 145, 220401.	1.2	1
210	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	1.2	1
211	Chemical physics of materials. Journal of Chemical Physics, 2020, 153, 100402.	1.2	0