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	Interplay of structural and dynamical heterogeneity in the nucleation mechanism in nickel. Faraday Discussions, 2022, 235, 406-415.	1.6	2
2	The role of structural order in heterogeneous ice nucleation. Chemical Science, 2022, 13, 5014-5026.	3.7	10
3	How do interfaces alter the dynamics of supercooled water?. Nanoscale, 2022, 14, 4254-4262.	2.8	4
4	General embedded cluster protocol for accurate modeling of oxygen vacancies in metal-oxides. Journal of Chemical Physics, 2022, 156, 124704.	1.2	9
5	Rapid Water Diffusion at Cryogenic Temperatures through an Inchworm-like Mechanism. Nano Letters, 2022, 22, 340-346.	4.5	5
6	Can molecular simulations reliably compare homogeneous and heterogeneous ice nucleation?. Journal of Chemical Physics, 2022, 156, 164501.	1.2	3
7	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
8	Water Flow in Single-Wall Nanotubes: Oxygen Makes It Slip, Hydrogen Makes It Stick. ACS Nano, 2022, 16, 10775-10782.	7.3	25
9	Observation and Characterization of Dicarbonyls on a RhCu Single-Atom Alloy. Journal of Physical Chemistry Letters, 2022, 13, 6316-6322.	2.1	2
10	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
11	Microscopic Kinetics Pathway of Salt Crystallization in Graphene Nanocapillaries. Physical Review Letters, 2021, 126, 136001.	2.9	22
12	First-principles design of a single-atomâ€“alloy propane dehydrogenation catalyst. Science, 2021, 372, 1444-1447.	6.0	185
13	Chemical physics software. Journal of Chemical Physics, 2021, 155, 010401.	1.2	2
14	Defect-Dependent Corrugation in Graphene. Nano Letters, 2021, 21, 8143-8150.	4.5	29
15	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
16	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
17	Periodic Trends in Adsorption Energies around Single-Atom Alloy Active Sites. Journal of Physical Chemistry Letters, 2021, 12, 10060-10067.	2.1	16
18	Water/oil interfacial tension reduction â€“ an interfacial entropy driven process. Physical Chemistry Chemical Physics, 2021, 23, 25075-25085.	1.3	17

#	Article	IF	Citations
19	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	1.2	1
20	Predicting heterogeneous ice nucleation with a data-driven approach. Nature Communications, 2020, 11, 4777.	5.8	35
21	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	1.2	2
22	The color center singlet state of oxygen vacancies in TiO2. Journal of Chemical Physics, 2020, 153, 204704.	1.2	13
23	An accurate and transferable machine learning potential for carbon. Journal of Chemical Physics, 2020, 153, 034702.	1.2	137
24	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
25	Chemical physics of materials. Journal of Chemical Physics, 2020, 153, 100402.	1.2	0
26	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> in Water: Bifurcated Hydrogen Bonding Structures and Fast Rotational Dynamics. Physical Review Letters, 2020, 125, 106001.	2.9	17
27	Electronic structure software. Journal of Chemical Physics, 2020, 153, 070401.	1.2	34
28	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> (110). Physical Review B, 2020, 101, .	1.1	15
29	Origins of fast diffusion of water dimers on surfaces. Nature Communications, 2020, 11, 1689.	5.8	39
30	Cation-controlled wetting properties of vermiculite membranes and its promise for fouling resistant oilâ€“water separation. Nature Communications, 2020, 11, 1097.	5.8	89
31	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
32	One-Dimensional Pnictogen Allotropes inside Single-Wall Carbon Nanotubes. Inorganic Chemistry, 2019, 58, 15216-15224.	1.9	18
33	Interaction between water and carbon nanostructures: How good are current density functional approximations?. Journal of Chemical Physics, 2019, 151, 164702.	1.2	47
34	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
35	Strain Relief during Ice Growth on a Hexagonal Template. Journal of the American Chemical Society, 2019, 141, 8599-8607.	6.6	24
36	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

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37	The quantum nature of hydrogen. International Reviews in Physical Chemistry, 2019, 38, 35-61.	0.9	18
38	Anomalously Low Barrier for Water Dimer Diffusion on Cu(111). Nano Letters, 2019, 19, 3049-3056.	4.5	20
39	Surface premelting of water ice. Nature Reviews Chemistry, 2019, 3, 172-188.	13.8	142
40	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
41	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
42	Elucidating the Stability and Reactivity of Surface Intermediates on Single-Atom Alloy Catalysts. ACS Catalysis, 2018, 8, 5038-5050.	5.5	152
43	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
44	Development of a machine learning potential for graphene. Physical Review B, 2018, 97, .	1.1	142
45	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
46	Pt/Cu single-atom alloys as coke-resistant catalysts for efficient Câ€“H activation. Nature Chemistry, 2018, 10, 325-332.	6.6	472
47	Carbon Monoxide Poisoning Resistance and Structural Stability of Single Atom Alloys. Topics in Catalysis, 2018, 61, 428-438.	1.3	117
48	Sticky when wet. Nature Chemistry, 2018, 10, 376-377.	6.6	2
49	Oneâ€Dimensional Arsenic Allotropes: Polymerization of Yellow Arsenic Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie, 2018, 130, 11823-11827.	1.6	2
50	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
51	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
52	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
53	Oneâ€Dimensional Arsenic Allotropes: Polymerization of Yellow Arsenic Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie - International Edition, 2018, 57, 11649-11653.	7.2	23
54	Unravelling the origins of ice nucleation on organic crystals. Chemical Science, 2018, 9, 8077-8088.	3.7	43

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55	Visualization of Water-Induced Surface Segregation of Polarons on Rutile TiO₂(110). Journal of Physical Chemistry Letters, 2018, 9, 4865-4871.	2.1	28
56	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
57	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
58	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
59	Encapsulation and Polymerization of White Phosphorus Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie, 2017, 129, 8256-8260.	1.6	26
60	Encapsulation and Polymerization of White Phosphorus Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie - International Edition, 2017, 56, 8144-8148.	7.2	70
61	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
62	Double-layer ice from first principles. Physical Review B, 2017, 95, .	1.1	29
63	How strongly do hydrogen and water molecules stick to carbon nanomaterials?. Journal of Chemical Physics, 2017, 146, .	1.2	38
64	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
65	Active sites in heterogeneous ice nucleationâ€”the example of K-rich feldspars. Science, 2017, 355, 367-371.	6.0	231
66	What makes a good descriptor for heterogeneous ice nucleation on OH-patterned surfaces. Physical Review B, 2017, 96, .	1.1	43
67	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
68	Simultaneous Deep Tunneling and Classical Hopping for Hydrogen Diffusion on Metals. Physical Review Letters, 2017, 119, 126001.	2.9	46
69	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
70	Hydrogenation Facilitates Proton Transfer through Two-Dimensional Honeycomb Crystals. Journal of Physical Chemistry Letters, 2017, 8, 6009-6014.	2.1	51
71	Structure of a model TiO2Âphotocatalytic interface. Nature Materials, 2017, 16, 461-466.	13.3	234
72	Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives. Journal of Chemical Physics, 2017, 147, 164113.	1.2	25

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73	Pre-critical fluctuations and what they disclose about heterogeneous crystal nucleation. Nature Communications, 2017, 8, 2257.	5.8	55
74	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
75	Editorial: The Future of Chemical Physics Conference 2016. Journal of Chemical Physics, 2016, 145, 220401.	1.2	1
76	Perspective: How good is DFT for water?. Journal of Chemical Physics, 2016, 144, 130901.	1.2	571
77	Ice formation on kaolinite: Insights from molecular dynamics simulations. Journal of Chemical Physics, 2016, 145, 211927.	1.2	53
78	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
79	Evidence for stable square ice from quantum Monte Carlo. Physical Review B, 2016, 94, .	1.1	46
80	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
81	Crystal Nucleation in Liquids: Open Questions and Future Challenges in Molecular Dynamics Simulations. Chemical Reviews, 2016, 116, 7078-7116.	23.0	635
82	Water at Interfaces. Chemical Reviews, 2016, 116, 7698-7726.	23.0	536
83	Inverse Temperature Dependence of Nuclear Quantum Effects in DNA Base Pairs. Journal of Physical Chemistry Letters, 2016, 7, 2125-2131.	2.1	46
84	Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges. Chemical Reviews, 2016, 116, 7529-7550.	23.0	439
85	Slippery when narrow. Nature, 2016, 537, 171-172.	13.7	24
86	Boosting the accuracy and speed of quantum Monte Carlo: Size consistency and time step. Physical Review B, 2016, 93, .	1.1	54
87	Toward Accurate Adsorption Energetics on Clay Surfaces. Journal of Physical Chemistry C, 2016, 120, 26402-26413.	1.5	30
88	Preparation, Structure, and Surface Chemistry of Niâ€“Au Single Atom Alloys. Journal of Physical Chemistry C, 2016, 120, 13574-13580.	1.5	70
89	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
90	A Blue-Sky Approach to Understanding Cloud Formation. Bulletin of the American Meteorological Society, 2016, 97, 1797-1802.	1.7	14

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91	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
92	Controlling Hydrogen Activation, Spillover, and Desorption with Pdâ€“Au Single-Atom Alloys. Journal of Physical Chemistry Letters, 2016, 7, 480-485.	2.1	169
93	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
94	Atomic-Scale Picture of the Composition, Decay, and Oxidation of Two-Dimensional Radioactive Films. ACS Nano, 2016, 10, 2152-2158.	7.3	5
95	Two Dimensional Ice from First Principles: Structures and Phase Transitions. Physical Review Letters, 2016, 116, 025501.	2.9	167
96	Fast diffusion of water nanodroplets on graphene. Nature Materials, 2016, 15, 66-71.	13.3	156
97	Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. Journal of Chemical Physics, 2015, 143, 102601.	1.2	10
98	Molecular simulations of heterogeneous ice nucleation. I. Controlling ice nucleation through surface hydrophilicity. Journal of Chemical Physics, 2015, 142, 184704.	1.2	122
99	Understanding corrosion inhibition with van der Waals DFT methods: the case of benzotriazole. Faraday Discussions, 2015, 180, 439-458.	1.6	60
100	Enhancement of low-energy electron emission in 2D radioactive films. Nature Materials, 2015, 14, 904-907.	13.3	30
101	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
102	Corrosion control: general discussion. Faraday Discussions, 2015, 180, 543-576.	1.6	12
103	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
104	Molecular simulations of heterogeneous ice nucleation. II. Peeling back the layers. Journal of Chemical Physics, 2015, 142, 184705.	1.2	72
105	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. Journal of Chemical Physics, 2015, 142, 181101.	1.2	56
106	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
107	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
108	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

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109	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
110	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
111	Solvent-Induced Proton Hopping at a Waterâ€“Oxide Interface. Journal of Physical Chemistry Letters, 2014, 5, 474-480.	2.1	82
112	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
113	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
114	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
115	Significant Quantum Effects in Hydrogen Activation. ACS Nano, 2014, 8, 4827-4835.	7.3	44
116	Nature of proton transport in a water-filled carbon nanotube and in liquid water. Physical Chemistry Chemical Physics, 2013, 15, 6344.	1.3	51
117	The microscopic features of heterogeneous ice nucleation may affect the macroscopic morphology of atmospheric ice crystals. Faraday Discussions, 2013, 167, 389.	1.6	80
118	The role of van der Waals forces in water adsorption on metals. Journal of Chemical Physics, 2013, 138, 024708.	1.2	173
119	Quantum Effects in the Diffusion of Hydrogen on Ru(0001). Journal of Physical Chemistry Letters, 2013, 4, 1565-1569.	2.1	59
120	Understanding the role of ions and water molecules in the NaCl dissolution process. Journal of Chemical Physics, 2013, 139, 234702.	1.2	40
121	Quantum simulation of low-temperature metallic liquid hydrogen. Nature Communications, 2013, 4, 2064.	5.8	75
122	Classical and quantum ordering of protons in cold solid hydrogen under megabar pressures. Journal of Physics Condensed Matter, 2013, 25, 085402.	0.7	25
123	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
124	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
125	Hydrogen-bonded assembly of methanol on Cu(111). Physical Chemistry Chemical Physics, 2012, 14, 11846.	1.3	28
126	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

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127	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
128	Improved description of soft layered materials with van der Waals density functional theory. Journal of Physics Condensed Matter, 2012, 24, 424216.	0.7	150
129	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. Physical Review B, 2012, 86, .	1.1	243
130	Water-hydroxyl phases on an open metal surface: breaking the ice rules. Chemical Science, 2012, 3, 93-102.	3.7	45
131	Non-hexagonal ice at hexagonal surfaces: the role of lattice mismatch. Physical Chemistry Chemical Physics, 2012, 14, 7944.	1.3	53
132	A molecular perspective of water at metal interfaces. Nature Materials, 2012, 11, 667-674.	13.3	568
133	Initial stages of salt crystal dissolution determined with ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2011, 13, 13162.	1.3	51
134	Trends in water monomer adsorption and dissociation on flat insulating surfaces. Physical Chemistry Chemical Physics, 2011, 13, 12447.	1.3	40
135	Acetone adsorption on ice investigated by X-ray spectroscopy and density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 19988.	1.3	32
136	Theory of gold on ceria. Physical Chemistry Chemical Physics, 2011, 13, 22-33.	1.3	108
137	<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) TjETQq1 1 0.78431 by Bjerrum Defects. Physical Review Letters, 2011, 106, 046103.	2.5	0
138	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
139	Proton ordering in cubic ice and hexagonal ice; a potential new ice phaseâ€”XIc. Physical Chemistry Chemical Physics, 2011, 13, 19788.	1.3	60
140	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	2.9	193
141	Binding of hydrogen on benzene, coronene, and graphene from quantum Monte Carlo calculations. Journal of Chemical Physics, 2011, 134, 134701.	1.2	48
142	Adsorption and diffusion of water on graphene from first principles. Physical Review B, 2011, 84, .	1.1	218
143	The Energy of Hydroxyl Coadsorbed with Water on Pt(111). Journal of Physical Chemistry C, 2011, 115, 23008-23012.	1.5	45
144	Visualization of Hydrogen Bonding and Associated Chirality in Methanol Hexamers. Physical Review Letters, 2011, 107, 256101.	2.9	42

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145	Melting the Ice: On the Relation between Melting Temperature and Size for Nanoscale Ice Crystals. ACS Nano, 2011, 5, 4562-4569.	7.3	65
146	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
147	Van der Waals density functionals applied to solids. Physical Review B, 2011, 83, .	1.1	3,608
148	Large variation of vacancy formation energies in the surface of crystalline ice. Nature Materials, 2011, 10, 794-798.	13.3	59
149	Quantum nuclear effects on the location of hydrogen above and below the palladium (100) surface. Surface Science, 2011, 605, 689-694.	0.8	13
150	The kaolinite (001) polar basal plane. Surface Science, 2010, 604, 111-117.	0.8	30
151	Dynamics of quantum tunneling: Effects on the rate and transition path of OH on Cu(110). Physical Review B, 2010, 81, .	1.1	14
152	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
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	Quantum Nature of the Proton in Water-Hydroxyl Overlayers on Metal Surfaces. Physical Review Letters, 2010, 104, 066102.	2.9	101
155	Chemical accuracy for the van der Waals density functional. Journal of Physics Condensed Matter, 2010, 22, 022201.	0.7	2,222
156	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
157	Proton transfer in adsorbed water dimers. Physical Chemistry Chemical Physics, 2010, 12, 3953.	1.3	28
158	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
159	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> (110). Physical Review B, 2010, 82, .	1.1	182
160	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
161	Local Investigation of Femtosecond Laser Induced Dynamics of Water Nanoclusters on Cu(111). Physical Review Letters, 2009, 103, 026101.	2.9	37
162	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

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163	A one-dimensional ice structure built from pentagons. Nature Materials, 2009, 8, 427-431.	13.3	212
164	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
165	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
166	Experimental and theoretical study of oxygen adsorption structures on Ag(111). Physical Review B, 2009, 80, .	1.1	90
167	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
168	On thin ice: surface order and disorder during pre-melting. Faraday Discussions, 2009, 141, 277-292.	1.6	40
169	The water-benzene interaction: Insight from electronic structure theories. Journal of Chemical Physics, 2009, 130, 154303.	1.2	73
170	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:mrow materials. Physical Review B, 2009, 80, .	1.1	422
171	How strong is the bond between water and salt?. Surface Science, 2008, 602, L135-L138.	0.8	21
172	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
173	Manipulation and Control of Hydrogen Bond Dynamics in Absorbed Ice Nanoclusters. Physical Review Letters, 2008, 101, 136102.	2.9	64
174	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
175	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
176	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
177	Structure of gold atoms on stoichiometric and defective ceria surfaces. Journal of Chemical Physics, 2008, 129, 194708.	1.2	103
178	Simulating ice nucleation, one molecule at a time, with the â€˜DFT microscopeâ€™. Faraday Discussions, 2007, 136, 287.	1.6	42
179	Density functional theory study of flat and stepped NaCl(001). Physical Review B, 2007, 76, .	1.1	40
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