Angelos Michaelides

List of Publications by Citations

200 papers	20,582 citations	68 h-index	140 g-index
218 ext. papers	23,042 ext. citations	8.4 avg, IF	7.39 L-index

#	Paper	IF	Citations
200	Van der Waals density functionals applied to solids. *Physical Review B*, **2011**, 83,	3.3	2972
199	Chemical accuracy for the van der Waals density functional. *Journal of Physics Condensed Matter*, **2010**, 22, 022201	1.8	1759
198	Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory. *Journal of Chemical Physics*, **2012**, 137, 120901	3.9	813
197	A molecular perspective of water at metal interfaces. *Nature Materials*, **2012**, 11, 667-74	27	472
196	Identification of general linear relationships between activation energies and enthalpy changes for dissociation reactions at surfaces. *Journal of the American Chemical Society*, **2003**, 125, 3704-5	16.4	452
195	Perspective: How good is DFT for water?. *Journal of Chemical Physics*, **2016**, 144, 130901	3.9	451
194	Crystal Nucleation in Liquids: Open Questions and Future Challenges in Molecular Dynamics Simulations. *Chemical Reviews*, **2016**, 116, 7078-116	68.1	430
193	Water at Interfaces. *Chemical Reviews*, **2016**, 116, 7698-726	68.1	388
192	Stone-Wales defects in graphene and other planar sp2-bonded materials. *Physical Review B*, **2009**, 80,	3.3	359
191	Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges. *Chemical Reviews*, **2016**, 116, 7529-50	68.1	324
190	General model for water monomer adsorption on close-packed transition and noble metal surfaces. *Physical Review Letters*, **2003**, 90, 216102	7.4	321
189	Pt/Cu single-atom alloys as coke-resistant catalysts for efficient C-H activation. *Nature Chemistry*, **2018**, 10, 325-332	17.6	308
188	Quantum nature of the hydrogen bond. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 6369-6373	11.5	297
187	Catalytic water formation on platinum: a first-principles study. *Journal of the American Chemical Society*, **2001**, 123, 4235-42	16.4	281
186	Ice nanoclusters at hydrophobic metal surfaces. *Nature Materials*, **2007**, 6, 597-601	27	257
185	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, 6872-7	11.5	256
184	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. *Physical Review B*, **2012**, 86,	3.3	227

183	Different surface chemistries of water on Ru[0001]: from monomer adsorption to partially dissociated bilayers. *Journal of the American Chemical Society*, **2003**, 125, 2746-55	16.4	209
182	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	3.9	204
181	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	3.9	195
180	Structure of a model TiO photocatalytic interface. *Nature Materials*, **2017**, 16, 461-466	27	188
179	Adsorption and diffusion of water on graphene from first principles. *Physical Review B*, **2011**, 84,	3.3	188
178	Atomistic details of oxide surfaces and surface oxidation: the example of copper and its oxides. *Surface Science Reports*, **2015**, 70, 424-447	12.9	187
177	Hydrogen bonds and van der waals forces in ice at ambient and high pressures. *Physical Review Letters*, **2011**, 107, 185701	7.4	181
176	A one-dimensional ice structure built from pentagons. *Nature Materials*, **2009**, 8, 427-31	27	178
175	Active sites in heterogeneous ice nucleation-the example of K-rich feldspars. *Science*, **2017**, 355, 367-371	33.3	170
174	Structure and dynamics of liquid water on rutile TiO2(110). *Physical Review B*, **2010**, 82,	3.3	162
173	A density functional theory study of hydroxyl and the intermediate in the water formation reaction on Pt. *Journal of Chemical Physics*, **2001**, 114, 513	3.9	161
172	Novel water overlayer growth on Pd(111) characterized with scanning tunneling microscopy and density functional theory. *Physical Review Letters*, **2004**, 93, 116101	7.4	159
171	Insight into H2O-ice adsorption and dissociation on metal surfaces from first-principles simulations. *Physical Review B*, **2004**, 69,	3.3	156
170	The role of van der Waals forces in water adsorption on metals. *Journal of Chemical Physics*, **2013**, 138, 024708	3.9	155
169	To wet or not to wet? Dispersion forces tip the balance for water ice on metals. *Physical Review Letters*, **2011**, 106, 026101	7.4	151
168	Insight into the description of van der Waals forces for benzene adsorption on transition metal (111) surfaces. *Journal of Chemical Physics*, **2014**, 140, 084704	3.9	149
167	The Many Faces of Heterogeneous Ice Nucleation: Interplay Between Surface Morphology and Hydrophobicity. *Journal of the American Chemical Society*, **2015**, 137, 13658-69	16.4	147
166	Improved description of soft layered materials with van der Waals density functional theory. *Journal of Physics Condensed Matter*, **2012**, 24, 424216	1.8	134

165	Density functional theory simulations of water–metal interfaces: waltzing waters, a novel 2D ice phase, and more. *Applied Physics A: Materials Science and Processing*, **2006**, 85, 415-425	2.6	134
164	Water on the hydroxylated (001) surface of kaolinite: From monomer adsorption to a flat 2D wetting layer. *Surface Science*, **2008**, 602, 960-974	1.8	133
163	Insight into Microscopic Reaction Pathways in Heterogeneous Catalysis. *Journal of the American Chemical Society*, **2000**, 122, 9866-9867	16.4	131
162	Controlling Hydrogen Activation, Spillover, and Desorption with Pd-Au Single-Atom Alloys. *Journal of Physical Chemistry Letters*, **2016**, 7, 480-5	6.4	129
161	Two Dimensional Ice from First Principles: Structures and Phase Transitions. *Physical Review Letters*, **2016**, 116, 025501	7.4	129
160	Revisiting the structure of the p(4 x 4) surface oxide on Ag(111). *Physical Review Letters*, **2006**, 96, 146101	7.4	127
159	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	6.4	127
158	Fast diffusion of water nanodroplets on graphene. *Nature Materials*, **2016**, 15, 66-71	27	119
157	Resolution of an ancient surface science anomaly: work function change induced by N adsorption on W [100]. *Physical Review Letters*, **2003**, 90, 246103	7.4	112
156	Structures and thermodynamic phase transitions for oxygen and silver oxide phases on Ag{1 1 1}. *Chemical Physics Letters*, **2003**, 367, 344-350	2.5	109
155	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	3.9	107
154	Positive charge States and possible polymorphism of gold nanoclusters on reduced ceria. *Journal of the American Chemical Society*, **2010**, 132, 2175-82	16.4	104
153	Molecular simulations of heterogeneous ice nucleation. I. Controlling ice nucleation through surface hydrophilicity. *Journal of Chemical Physics*, **2015**, 142, 184704	3.9	100
152	New insights into ethene epoxidation on two oxidized Ag[111] surfaces. *Journal of the American Chemical Society*, **2003**, 125, 5620-1	16.4	100
151	Oxygen vacancy clusters on ceria: Decisive role of cerium f electrons. *Physical Review B*, **2009**, 79,	3.3	98
150	Theory of gold on ceria. *Physical Chemistry Chemical Physics*, **2011**, 13, 22-33	3.6	97
149	Structure of gold atoms on stoichiometric and defective ceria surfaces. *Journal of Chemical Physics*, **2008**, 129, 194708	3.9	97
148	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	2.9	97

147	Water dimer diffusion on Pd[111] assisted by an H-bond donor-acceptor tunneling exchange. *Physical Review Letters*, **2004**, 92, 136104	7.4	96
146	Elucidating the Stability and Reactivity of Surface Intermediates on Single-Atom Alloy Catalysts. *ACS Catalysis*, **2018**, 8, 5038-5050	13.1	95
145	Development of a machine learning potential for graphene. *Physical Review B*, **2018**, 97,	3.3	94
144	Quantum nature of the proton in water-hydroxyl overlayers on metal surfaces. *Physical Review Letters*, **2010**, 104, 066102	7.4	90
143	Physical origin of the high reactivity of subsurface hydrogen in catalytic hydrogenation. *Journal of Chemical Physics*, **1999**, 111, 1343-1345	3.9	88
142	Ice formation on kaolinite: Lattice match or amphoterism?. *Surface Science*, **2007**, 601, 5378-5381	1.8	87
141	Insight from first principles into the nature of the bonding between water molecules and 4d metal surfaces. *Journal of Chemical Physics*, **2009**, 130, 184707	3.9	84
140	Experimental and theoretical study of oxygen adsorption structures on Ag(111). *Physical Review B*, **2009**, 80,	3.3	80
139	Surface premelting of water ice. *Nature Reviews Chemistry*, **2019**, 3, 172-188	34.6	77
138	Methyl chemisorption on Ni(111) and CHM multicentre bonding: a density functional theory study. *Surface Science*, **1999**, 437, 362-376	1.8	76
137	Carbon Monoxide Poisoning Resistance and Structural Stability of Single Atom Alloys. *Topics in Catalysis*, **2018**, 61, 428-438	2.3	75
136	Solvent-Induced Proton Hopping at a Water-Oxide Interface. *Journal of Physical Chemistry Letters*, **2014**, 5, 474-480	6.4	75
135	Anchoring Sites for Initial Au Nucleation on CeO2{111}: O Vacancy versus Ce Vacancy. *Journal of Physical Chemistry C*, **2009**, 113, 6411-6417	3.8	73
134	The microscopic features of heterogeneous ice nucleation may affect the macroscopic morphology of atmospheric ice crystals. *Faraday Discussions*, **2013**, 167, 389-403	3.6	70
133	c(2⨯2) water-hydroxyl layer on Cu(110): a wetting layer stabilized by Bjerrum defects. *Physical Review Letters*, **2011**, 106, 046103	7.4	70
132	The water-benzene interaction: insight from electronic structure theories. *Journal of Chemical Physics*, **2009**, 130, 154303	3.9	67
131	Quantum simulation of low-temperature metallic liquid hydrogen. *Nature Communications*, **2013**, 4, 2064	17.4	65
130	Surface energy and surface proton order of ice Ih. *Physical Review Letters*, **2008**, 101, 155703	7.4	65

129	Molecular simulations of heterogeneous ice nucleation. II. Peeling back the layers. *Journal of Chemical Physics*, **2015**, 142, 184705	3.9	64
128	First-principles design of a single-atom□lloy propane dehydrogenation catalyst. *Science*, **2021**, 372, 1444-1447	3.9	62
127	Influence of water on the electronic structure of metal-supported graphene: Insights from van der Waals density functional theory. *Physical Review B*, **2012**, 85,	3.3	61
126	Preparation, Structure, and Surface Chemistry of Ni□u Single Atom Alloys. *Journal of Physical Chemistry C*, **2016**, 120, 13574-13580	3.8	60
125	The Carbon-Water Interface: Modeling Challenges and Opportunities for the Water-Energy Nexus. *Annual Review of Chemical and Biomolecular Engineering*, **2016**, 7, 533-56	8.9	60
124	Microscopic Mechanism and Kinetics of Ice Formation at Complex Interfaces: Zooming in on Kaolinite. *Journal of Physical Chemistry Letters*, **2016**, 7, 2350-5	6.4	59
123	Melting the ice: on the relation between melting temperature and size for nanoscale ice crystals. *ACS Nano*, **2011**, 5, 4562-9	16.7	59
122	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	3.9	57
121	Softened C□H modes of adsorbed methyl and their implications for dehydrogenation: An ab initio study. *Journal of Chemical Physics*, **2001**, 114, 2523-2526	3.9	56
120	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	11.5	55
119	Proton ordering in cubic ice and hexagonal ice; a potential new ice phase--XIc. *Physical Chemistry Chemical Physics*, **2011**, 13, 19788-95	3.6	55
118	Manipulation and control of hydrogen bond dynamics in absorbed ice nanoclusters. *Physical Review Letters*, **2008**, 101, 136102	7.4	53
117	Encapsulation and Polymerization of White Phosphorus Inside Single-Wall Carbon Nanotubes. *Angewandte Chemie - International Edition*, **2017**, 56, 8144-8148	16.4	52
116	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	11.5	52
115	Large variation of vacancy formation energies in the surface of crystalline ice. *Nature Materials*, **2011**, 10, 794-8	27	52
114	Density functional theory study of the interaction of monomeric water with the Ag{111} surface. *Physical Review B*, **2004**, 69,	3.3	51
113	Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods. *Journal of Physical Chemistry Letters*, **2019**, 10, 358-368	6.4	51
112	Quantum Effects in the Diffusion of Hydrogen on Ru(0001). *Journal of Physical Chemistry Letters*, **2013**, 4, 1565-1569	6.4	50

111	Non-hexagonal ice at hexagonal surfaces: the role of lattice mismatch. *Physical Chemistry Chemical Physics*, **2012**, 14, 7944-9	3.6	49
110	A critical assessment of theoretical methods for finding reaction pathways and transition states of surface processes. *Journal of Physics Condensed Matter*, **2010**, 22, 074203	1.8	49
109	A density functional theory study of CH2 and H adsorption on Ni(111). *Journal of Chemical Physics*, **2000**, 112, 6006-6014	3.9	49
108	An accurate and transferable machine learning potential for carbon. *Journal of Chemical Physics*, **2020**, 153, 034702	3.9	49
107	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. *Journal of Chemical Physics*, **2015**, 142, 181101	3.9	47
106	Nature of proton transport in a water-filled carbon nanotube and in liquid water. *Physical Chemistry Chemical Physics*, **2013**, 15, 6344-9	3.6	47
105	Understanding corrosion inhibition with van der Waals DFT methods: the case of benzotriazole. *Faraday Discussions*, **2015**, 180, 439-58	3.6	47
104	Formation of Methane Hydrate in the Presence of Natural and Synthetic Nanoparticles. *Journal of the American Chemical Society*, **2018**, 140, 3277-3284	16.4	46
103	A first principles study of CH3 dehydrogenation on Ni(111). *Journal of Chemical Physics*, **2000**, 112, 8120-8125	3.9	46
102	Hydrogenation of S to H2S on Pt(111): A first-principles study. *Journal of Chemical Physics*, **2001**, 115, 8570-8574	3.9	45
101	Binding of hydrogen on benzene, coronene, and graphene from quantum Monte Carlo calculations. *Journal of Chemical Physics*, **2011**, 134, 134701	3.9	44
100	Interfacial water: a first principles molecular dynamics study of a nanoscale water film on salt. *Journal of Chemical Physics*, **2009**, 130, 234702	3.9	44
99	Boosting the accuracy and speed of quantum Monte Carlo: Size consistency and time step. *Physical Review B*, **2016**, 93,	3.3	43
98	Water-hydroxyl phases on an open metal surface: breaking the ice rules. *Chemical Science*, **2012**, 3, 93-102	7.4	41
97	The Energy of Hydroxyl Coadsorbed with Water on Pt(111). *Journal of Physical Chemistry C*, **2011**, 115, 23008-23012	3.8	41
96	Visualization of hydrogen bonding and associated chirality in methanol hexamers. *Physical Review Letters*, **2011**, 107, 256101	7.4	41
95	Initial stages of salt crystal dissolution determined with ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2011**, 13, 13162-6	3.6	41
94	Density oscillations in a nanoscale water film on salt: insight from ab initio molecular dynamics. *Journal of the American Chemical Society*, **2008**, 130, 8572-3	16.4	39

93	Simulating ice nucleation, one molecule at a time, with the 'DFT microscope'. *Faraday Discussions*, **2007**, 136, 287-97; discussion 309-28	3.6	39
92	Stability of Complex Biomolecular Structures: van der Waals, Hydrogen Bond Cooperativity, and Nuclear Quantum Effects. *Journal of Physical Chemistry Letters*, **2015**, 6, 4233-8	6.4	38
91	Cooperative interplay of van der Waals forces and quantum nuclear effects on adsorption: H at graphene and at coronene. *ACS Nano*, **2014**, 8, 9905-13	16.7	38
90	Trends in water monomer adsorption and dissociation on flat insulating surfaces. *Physical Chemistry Chemical Physics*, **2011**, 13, 12447-53	3.6	38
89	Density functional theory study of flat and stepped NaCl(001). *Physical Review B*, **2007**, 76,	3.3	37
88	Ice formation on kaolinite: Insights from molecular dynamics simulations. *Journal of Chemical Physics*, **2016**, 145, 211927	3.9	37
87	Pre-critical fluctuations and what they disclose about heterogeneous crystal nucleation. *Nature Communications*, **2017**, 8, 2257	17.4	36
86	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	3.9	36
85	Significant quantum effects in hydrogen activation. *ACS Nano*, **2014**, 8, 4827-35	16.7	35
84	Surface energy and surface proton order of the ice Ih basal and prism surfaces. *Journal of Physics Condensed Matter*, **2010**, 22, 074209	1.8	35
83	On thin ice: surface order and disorder during pre-melting. *Faraday Discussions*, **2009**, 141, 277-92; discussion 309-46	3.6	35
82	Evidence for stable square ice from quantum Monte Carlo. *Physical Review B*, **2016**, 94,	3.3	35
81	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	3.8	35
80	Understanding the role of ions and water molecules in the NaCl dissolution process. *Journal of Chemical Physics*, **2013**, 139, 234702	3.9	34
79	First-principles study of H2O diffusion on a metal surface: H2O on Al{100}. *Physical Review B*, **2004**, 69,	3.3	34
78	Inverse Temperature Dependence of Nuclear Quantum Effects in DNA Base Pairs. *Journal of Physical Chemistry Letters*, **2016**, 7, 2125-31	6.4	34
77	Cation-controlled wetting properties of vermiculite membranes and its promise for fouling resistant oil-water separation. *Nature Communications*, **2020**, 11, 1097	17.4	33
76	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M(dobdc) Metal-Organic Frameworks. *Journal of Physical Chemistry A*, **2017**, 121, 4139-4151	2.8	32

75	Local investigation of femtosecond laser induced dynamics of water nanoclusters on Cu(111). *Physical Review Letters*, **2009**, 103, 026101	7.4	32
74	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	3.9	31
73	How strongly do hydrogen and water molecules stick to carbon nanomaterials?. *Journal of Chemical Physics*, **2017**, 146, 094701	3.9	31
72	Is High-Density Amorphous Ice Simply a "Derailed" State along the Ice I to Ice IV Pathway?. *Journal of Physical Chemistry Letters*, **2017**, 8, 1645-1650	6.4	31
71	What makes a good descriptor for heterogeneous ice nucleation on OH-patterned surfaces. *Physical Review B*, **2017**, 96,	3.3	31
70	Hydrogenation Facilitates Proton Transfer through Two-Dimensional Honeycomb Crystals. *Journal of Physical Chemistry Letters*, **2017**, 8, 6009-6014	6.4	31
69	Acetone adsorption on ice investigated by X-ray spectroscopy and density functional theory. *Physical Chemistry Chemical Physics*, **2011**, 13, 19988-96	3.6	31
68	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	3.9	31
67	Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. *Journal of Chemical Physics*, **2017**, 147, 044710	3.9	30
66	Simultaneous Deep Tunneling and Classical Hopping for Hydrogen Diffusion on Metals. *Physical Review Letters*, **2017**, 119, 126001	7.4	29
65	Proton transfer in adsorbed water dimers. *Physical Chemistry Chemical Physics*, **2010**, 12, 3953-6	3.6	28
64	Reply to Comment on 'Structure and dynamics of liquid water on rutile TiO2(110)' *Physical Review B*, **2012**, 85,	3.3	28
63	Unravelling the origins of ice nucleation on organic crystals. *Chemical Science*, **2018**, 9, 8077-8088	9.4	27
62	Hydrogen-bonded assembly of methanol on Cu(111). *Physical Chemistry Chemical Physics*, **2012**, 14, 11846-52	3.6	26
61	Water-Ice Analogues of Polycyclic Aromatic Hydrocarbons: Water Nanoclusters on Cu(111). *Journal of the American Chemical Society*, **2017**, 139, 6403-6410	16.4	25
60	Enhancement of low-energy electron emission in 2D radioactive films. *Nature Materials*, **2015**, 14, 904-7	27	25
59	The kaolinite (001) polar basal plane. *Surface Science*, **2010**, 604, 111-117	1.8	25
58	Toward Accurate Adsorption Energetics on Clay Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 26402-26413	3.8	24

57	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	3.9	24
56	Structure and energetics of hydrogen-bonded networks of methanol on close packed transition metal surfaces. *Journal of Chemical Physics*, **2014**, 141, 014701	3.9	24
55	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	3.9	24
54	Strong Coupling between Nanofluidic Transport and Interfacial Chemistry: How Defect Reactivity Controls Liquid-Solid Friction through Hydrogen Bonding. *Journal of Physical Chemistry Letters*, **2016**, 7, 1381-6	6.4	23
53	Classical and quantum ordering of protons in cold solid hydrogen under megabar pressures. *Journal of Physics Condensed Matter*, **2013**, 25, 085402	1.8	23
52	Origins of fast diffusion of water dimers on surfaces. *Nature Communications*, **2020**, 11, 1689	17.4	21
51	How strong is the bond between water and salt?. *Surface Science*, **2008**, 602, L135-L138	1.8	21
50	Encapsulation and Polymerization of White Phosphorus Inside Single-Wall Carbon Nanotubes. *Angewandte Chemie*, **2017**, 129, 8256-8260	3.6	20
49	Double-layer ice from first principles. *Physical Review B*, **2017**, 95,	3.3	20
48	Interaction between water and carbon nanostructures: How good are current density functional approximations?. *Journal of Chemical Physics*, **2019**, 151, 164702	3.9	20
47	Visualization of Water-Induced Surface Segregation of Polarons on Rutile TiO(110). *Journal of Physical Chemistry Letters*, **2018**, 9, 4865-4871	6.4	19
46	Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives. *Journal of Chemical Physics*, **2017**, 147, 164113	3.9	19
45	Predicting heterogeneous ice nucleation with a data-driven approach. *Nature Communications*, **2020**, 11, 4777	17.4	19
44	Strain Relief during Ice Growth on a Hexagonal Template. *Journal of the American Chemical Society*, **2019**, 141, 8599-8607	16.4	18
43	One-Dimensional Arsenic Allotropes: Polymerization of Yellow Arsenic Inside Single-Wall Carbon Nanotubes. *Angewandte Chemie - International Edition*, **2018**, 57, 11649-11653	16.4	18
42	Communication: ab initio simulations of hydrogen-bonded ferroelectrics: collective tunneling and the origin of geometrical isotope effects. *Journal of Chemical Physics*, **2014**, 140, 041103	3.9	18
41	Tuning dissociation using isoelectronically doped graphene and hexagonal boron nitride: Water and other small molecules. *Journal of Chemical Physics*, **2016**, 144, 154706	3.9	18
40	Initial stages in the oxidation and reduction of the 4□ surface oxide phase on Ag{111}: A combined density-functional theory and STM simulation study. *Physical Review B*, **2003**, 68,	3.3	17

39	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	3.9	17
38	Machine learning potentials for complex aqueous systems made simple. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	17
37	Nanoscience: Slippery when narrow. *Nature*, **2016**, 537, 171-2	50.4	16
36	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	11.5	13
35	Carbon Monoxide Mediated Hydrogen Release from PtCu Single-Atom Alloys: The Punctured Molecular Cork Effect. *Journal of Physical Chemistry C*, **2019**, 123, 10419-10428	3.8	13
34	Adsorption Behavior of Organic Molecules: A Study of Benzotriazole on Cu(111) with Spectroscopic and Theoretical Methods. *Langmuir*, **2019**, 35, 882-893	4	13
33	Heterogeneous seeded molecular dynamics as a tool to probe the ice nucleating ability of crystalline surfaces. *Journal of Chemical Physics*, **2018**, 149, 072327	3.9	13
32	A Blue-Sky Approach to Understanding Cloud Formation. *Bulletin of the American Meteorological Society*, **2016**, 97, 1797-1802	6.1	12
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	3.9	12
30	Dynamics of quantum tunneling: Effects on the rate and transition path of OH on Cu(110). *Physical Review B*, **2010**, 81,	3.3	12
29	Quantum nuclear effects on the location of hydrogen above and below the palladium (100) surface. *Surface Science*, **2011**, 605, 689-694	1.8	12
28	The quantum nature of hydrogen. *International Reviews in Physical Chemistry*, **2019**, 38, 35-61	7	11
27	Communication: Truncated non-bonded potentials can yield unphysical behavior in molecular dynamics simulations of interfaces. *Journal of Chemical Physics*, **2017**, 147, 121102	3.9	10
26	Corrosion control: general discussion. *Faraday Discussions*, **2015**, 180, 543-76	3.6	10
25	Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. *Journal of Chemical Physics*, **2015**, 143, 102601	3.9	10
24	"Textbook" adsorption at "nontextbook" adsorption sites: halogen atoms on alkali halide surfaces. *Physical Review Letters*, **2006**, 97, 046802	7.4	10
23	Microscopic Kinetics Pathway of Salt Crystallization in Graphene Nanocapillaries. *Physical Review Letters*, **2021**, 126, 136001	7.4	9
22	Chirality at two-dimensional surfaces: A perspective from small molecule alcohol assembly on Au(111). *Journal of Chemical Physics*, **2018**, 149, 034703	3.9	8

21	Machine Learning Potential for Hexagonal Boron Nitride Applied to Thermally and Mechanically Induced Rippling. *Journal of Physical Chemistry C*, **2020**, 124, 22278-22290	3.8	8
20	Anomalously Low Barrier for Water Dimer Diffusion on Cu(111). *Nano Letters*, **2019**, 19, 3049-3056	11.5	7
19	Small polarons and the Janus nature of TiO2(110). *Physical Review B*, **2020**, 101,	3.3	7
18	One-Dimensional Pnictogen Allotropes inside Single-Wall Carbon Nanotubes. *Inorganic Chemistry*, **2019**, 58, 15216-15224	5.1	7
17	The color center singlet state of oxygen vacancies in TiO. *Journal of Chemical Physics*, **2020**, 153, 204704	3.9	7
16	Hydration of NH_{4}^{+} in Water: Bifurcated Hydrogen Bonding Structures and Fast Rotational Dynamics. *Physical Review Letters*, **2020**, 125, 106001	7.4	6
15	Atomic-Scale Picture of the Composition, Decay, and Oxidation of Two-Dimensional Radioactive Films. *ACS Nano*, **2016**, 10, 2152-8	16.7	5
14	An Introduction to the Theory of Crystalline Elemental Solids and their Surfaces **2013**, 13-72		5
13	The unhappy marriage of transition and noble metal atoms: A new way to enhance catalytic activity? (A perspective on: When adding an unreactive metal enhances catalytic activity: NOx decomposition over silver rhodium bimetallic surfaces by O.R. Inderwildi, S.J. Jenkins, D.A. King). *Surface Science*, **2007**, 601, 3529-3531	1.8	5
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