Axel Gross

List of Publications by Year
in descending order

243 papers	12,270 citations	16411 64 h-index	32761 100 g-index
281 all docs	281 docs citations	281 times ranked	9348 citing authors

#	Article	IF	Citations
1	Six-Dimensional Quantum Dynamics of Adsorption and Desorption ofH2at Pd(100): Steering and Steric Effects. Physical Review Letters, 1995, 75, 2718-2721.	2.9	358
2	Reactions at surfaces studied by ab initio dynamics calculations. Surface Science Reports, 1998, 32, 291-340.	3.8	346
3	Surface Strain versus Substrate Interaction in Heteroepitaxial Metal Layers: Pt on Ru(0001). Physical Review Letters, 2003, 91, 016101.	2.9	316
4	Representing high-dimensional potential-energy surfaces for reactions at surfaces by neural networks. Chemical Physics Letters, 2004, 395, 210-215.	1.2	311
5	Microscopic properties of lithium, sodium, and magnesium battery anode materials related to possible dendrite growth. Journal of Chemical Physics, 2014, 141, 174710.	1.2	311
6	Properties of metalâ€“water interfaces studied from first principles. New Journal of Physics, 2009, 11, 125003.	1.2	284
7	Experimental analysis of charge redistribution dueÂto chemical bonding by high-resolution transmission electron microscopy. Nature Materials, 2011, 10, 209-215.	13.3	270
8	Self-diffusion barriers: possible descriptors for dendrite growth in batteries?. Energy and Environmental Science, 2018, 11, 3400-3407.	15.6	247
9	Adsorption of small aromatic molecules on the (111) surfaces of noble metals: A density functional theory study with semiempirical corrections for dispersion effects. Journal of Chemical Physics, 2010, 132, 224701.	1.2	210
10	Toward an Atomic-Scale Understanding of Electrochemical Interface Structure and Dynamics. Journal of the American Chemical Society, 2019, 141, 4777-4790.	6.6	193
11	Fluoride ion batteries: Theoretical performance, safety, toxicity, and a combinatorial screening of new electrodes. Journal of Fluorine Chemistry, 2016, 182, 76-90.	0.9	191
12	Reactivity of Bimetallic Systems Studied from First Principles. Topics in Catalysis, 2006, 37, 29-39.	1.3	189
13	Insight into Sodium Insertion and the Storage Mechanism in Hard Carbon. ACS Energy Letters, 2018, 3, 2851-2857.	8.8	171
14	Quantum Theory of Dissociative Chemisorption on Metal Surfaces. Accounts of Chemical Research, 2002, 35, 193-200.	7.6	165
15	Ab initioquantum and molecular dynamics of the dissociative adsorption of hydrogen on Pd(100). Physical Review B, 1998, 57, 2493-2506.	1.1	158
16	Dissociative adsorption of hydrogen on strained Cu surfaces. Surface Science, 2003, 525, 107-118.	0.8	147
17	High-Dimensional Quantum Dynamics of Adsorption and Desorption ofH2at Cu(111). Physical Review Letters, 1994, 73, 3121-3124.	2.9	145
18	Dispersive interactions in water bilayers at metallic surfaces: A comparison of the PBE and RPBE functional including semiempirical dispersion corrections. Journal of Computational Chemistry, 2012, 33, 695-701.	1.5	136

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19	Challenges in the first-principles description of reactions in electrocatalysis. Catalysis Today, 2011, 165, 129-137.	2.2	135
20	A Thin and Uniform Fluoride-Based Artificial Interphase for the Zinc Metal Anode Enabling Reversible Zn/MnO₂ Batteries. ACS Energy Letters, 2021, 6, 3063-3071.	8.8	134
21	Local reactivity of metal overlayers: Density functional theory calculations of Pd on Au. Physical Review B, 2003, 67, .	1.1	130
22	Local reactivity of thin Pd overlayers on Au single crystals. Journal of Electroanalytical Chemistry, 2003, 548, 121-130.	1.9	129
23	The electric double layer at metal-water interfaces revisited based on a charge polarization scheme. Journal of Chemical Physics, 2018, 149, 084705.	1.2	128
24	The structure of water at a Pt(111) electrode and the potential of zero charge studied from first principles. Journal of Chemical Physics, 2016, 144, 194701.	1.2	127
25	Operando pH Measurements Decipher H⁺/Zn²⁺ Intercalation Chemistry in High-Performance Aqueous Zn/Î´-V₂O₅ Batteries. ACS Energy Letters, 2020, 5, 2979-2986.	8.8	126
26	Theoretical Surface Science. , 2009, , .		120
27	Strain and coordination effects in the adsorption properties of early transition metals: A density-functional theory study. Physical Review B, 2010, 81, .	1.1	119
28	The Importance of the Electrochemical Environment in the Electro-Oxidation of Methanol on Pt(111). ACS Catalysis, 2016, 6, 5575-5586.	5.5	117
29	Descriptions of surface chemical reactions using a neural network representation of the potential-energy surface. Physical Review B, 2006, 73, .	1.1	113
30	Water bilayer on the Pd/Au(111) overlayer system: Coadsorption and electric field effects. Chemical Physics Letters, 2005, 409, 157-162.	1.2	110
31	Change of the work function of platinum electrodes induced by halide adsorption. Beilstein Journal of Nanotechnology, 2014, 5, 152-161.	1.5	107
32	Hydrogen Dissociation Dynamics on Precovered Pd Surfaces: Langmuir is Still Right. Physical Review Letters, 2007, 98, 206107.	2.9	105
33	Density functional theory study of the electrochemical interface between a Pt electrode and an aqueous electrolyte using an implicit solvent method. Journal of Chemical Physics, 2015, 142, 234107.	1.2	103
34	Density functional theory study of the partial oxidation of methanol on copper surfaces. Journal of Catalysis, 2005, 231, 420-429.	3.1	102
35	Dispersion corrected RPBE studies of liquid water. Journal of Chemical Physics, 2014, 141, 064501.	1.2	102
36	Toward the Microscopic Identification of Anions and Cations at the Ionic Liquid|Ag(111) Interface: A Combined Experimental and Theoretical Investigation. ACS Nano, 2013, 7, 7773-7784.	7.3	100

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37	Local density of states effects at the metal-molecule interfaces in a molecular device. Nature Materials, 2006, 5, 394-399.	13.3	98
38	Numerically stable solution of coupled channel equations: The local reflection matrix. European Physical Journal B, 1993, 93, 91-101.	0.6	95
39	Tuning catalytic properties of bimetallic surfaces: Oxygen adsorption on pseudomorphic Pt/Ru overlayers. Electrochimica Acta, 2007, 52, 2219-2228.	2.6	93
40	Modelling the electric double layer at electrode/electrolyte interfaces. Current Opinion in Electrochemistry, 2019, 14, 1-6.	2.5	93
41	Structure of water layers on hydrogen-covered Pt electrodes. Catalysis Today, 2013, 202, 183-190.	2.2	90
42	Hydrogen adsorption on an open metal surface:H2/Pd(210). Physical Review B, 2002, 65, .	1.1	86
43	The role of lateral surface corrugation for the quantum dynamics of dissociative adsorption and associative desorption. Journal of Chemical Physics, 1995, 102, 5045-5058.	1.2	81
44	Periodic Density-Functional Calculations on Work-Function Change Induced by Adsorption of Halogens on Cu(111). Physical Review Letters, 2013, 110, 156804.	2.9	81
45	Water Structures at Metal Electrodes Studied by Ab Initio Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2014, 161, E3015-E3020.	1.3	81
46	FAIR data enabling new horizons for materials research. Nature, 2022, 604, 635-642.	13.7	81
47	CO adsorption on Cuâ€“Pd alloy surfaces: ligand versus ensemble effects. Physical Chemistry Chemical Physics, 2007, 9, 2216-2225.	1.3	79
48	The virtual chemistry lab for reactions at surfaces: Is it possible? Will it be useful?. Surface Science, 2002, 500, 347-367.	0.8	78
49	Influence of water on elementary reaction steps in electrocatalysis. Faraday Discussions, 2008, 140, 233-244.	1.6	78
50	Fingerprints for Spin-Selection Rules in the Interaction Dynamics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>at Al(111). Physical Review Letters, 2008, 101, 096104.	2.9	76
51	Concentration and Coverage Dependent Adlayer Structures: From Two-Dimensional Networks to Rotation in a Bearing. Journal of Physical Chemistry C, 2010, 114, 1268-1277.	1.5	76
52	Reaction dynamics of molecular hydrogen on silicon surfaces. Physical Review B, 1996, 54, 5978-5991.	1.1	75
53	Local reactivity of supported metal clusters: Pd n on Au(1 1 1). Surface Science, 2004, 559, L180-L186.	0.8	75
54	Total Oxidation of Methanol on Cu(110):Â A Density Functional Theory Study. Journal of Physical Chemistry A, 2007, 111, 8814-8822.	1.1	74

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55	First-principles study of the water structure on flat and stepped gold surfaces. Surface Science, 2012, 606, 886-891.	0.8	74
56	Signatures of nonadiabatic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>O</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> at Al(111): First-principles fewest-switches study. Physical Review B, 2010, 81, .	1.1	73
57	Equilibrium coverage of halides on metal electrodes. Surface Science, 2015, 631, 17-22.	0.8	72
58	Ab Initio Simulations of Water/Metal Interfaces. Chemical Reviews, 2022, 122, 10746-10776.	23.0	72
59	Coexistence of Atomic and Molecular Chemisorption States:H2/Pd(210). Physical Review Letters, 2001, 87, 096103.	2.9	70
60	Unified picture of the molecular adsorption process: O2/Pt(111). Surface Science, 2003, 539, L542-L548.	0.8	70
61	Theoretical Surface Science. Advanced Texts in Physics, 2003, , .	0.5	69
62	Interaction of a Self-Assembled Ionic Liquid Layer with Graphite(0001): A Combined Experimental and Theoretical Study. Journal of Physical Chemistry Letters, 2016, 7, 226-233.	2.1	68
63	Ab InitioMolecular Dynamics Study of the Desorption ofD2from Si(100). Physical Review Letters, 1997, 79, 701-704.	2.9	67
64	Trends in the chemical reactivity of surfaces studied byab initioquantum-dynamics calculations. Physical Review B, 1999, 59, 13297-13300.	1.1	67
65	Hydrogen and halide co-adsorption on Pt(111) in an electrochemical environment: a computational perspective. Electrochimica Acta, 2016, 216, 152-159.	2.6	66
66	Influence of molecular vibrations on dissociative adsorption. Chemical Physics Letters, 1996, 256, 417-423.	1.2	65
67	Water structures on a Pt(111) electrode from ab initio molecular dynamic simulations for a variety of electrochemical conditions. Physical Chemistry Chemical Physics, 2020, 22, 10431-10437.	1.3	65
68	Adsorption at Nanostructured Surfaces from First Principles. Journal of Computational and Theoretical Nanoscience, 2008, 5, 894-922.	0.4	63
69	Hierarchical Interactions and Their Influence upon the Adsorption of Organic Molecules on a Graphene Film. Journal of the American Chemical Society, 2011, 133, 9208-9211.	6.6	58
70	Role of zero-point effects in catalytic reactions involving hydrogen. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1997, 15, 1624-1629.	0.9	57
71	Detailed balance and phonon assisted sticking in adsorption and desorption of H2/Si. European Physical Journal B, 1994, 96, 231-234.	0.6	54
72	Halide adsorption on close-packed metal electrodes. Physical Chemistry Chemical Physics, 2014, 16, 13630-13634.	1.3	54

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73	Insights into the electrochemical processes of rechargeable magnesiumâ€“sulfur batteries with a new cathode design. Journal of Materials Chemistry A, 2019, 7, 25490-25502.	5.2	53
74	AbÂInitioMolecular Dynamics Study of Hot Atom Dynamics after Dissociative Adsorption of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>on Pd(100). Physical Review Letters, 2009, 103, 246101.	2.9	52
75	Hydrogen adsorption energies on bimetallic overlayer systems at the solidâ€“vacuum and the solidâ€“liquid interface. Surface Science, 2005, 597, 42-50.	0.8	50
76	Adsorption of 4-Mercaptopyridine on Au(111): A Periodic DFT Study. Langmuir, 2008, 24, 13985-13992.	1.6	50
77	Poisoning of hydrogen dissociation at Pd (100) by adsorbed sulfur studied by ab-initio quantum dynamics and ab-initio molecular dynamics. Surface Science, 1998, 416, L1095-L1100.	0.8	49
78	Some challenges in the first-principles modeling of structures and processes in electrochemical energy storage and transfer. Journal of Power Sources, 2015, 275, 531-538.	4.0	49
79	Tailoring the reactivity of bimetallic overlayer and surface alloy systems. Journal of Physics Condensed Matter, 2009, 21, 084205.	0.7	48
80	Ab Initio Molecular Dynamics Simulations of the Adsorption of H₂ on Palladium Surfaces. ChemPhysChem, 2010, 11, 1374-1381.	1.0	48
81	Cation Overcrowding Effect on the Oxygen Evolution Reaction. Jacs Au, 2021, 1, 1752-1765.	3.6	48
82	Hydrogen dissociation on metal surfaces - a model system for reactions on surfaces. Applied Physics A: Materials Science and Processing, 1998, 67, 627-635.	1.1	47
83	Dynamical quantum processes of molecular beams at surfaces: dissociative adsorption of hydrogen on metal surfaces. Surface Science, 1996, 363, 1-10.	0.8	46
84	Investigation on the formation of Mg metal anode/electrolyte interfaces in Mg/S batteries with electrolyte additives. Journal of Materials Chemistry A, 2020, 8, 22998-23010.	5.2	46
85	Structure and local reactivity of PdAg/Pd(111) surface alloys. Physical Chemistry Chemical Physics, 2013, 15, 1497-1508.	1.3	45
86	Steering and ro-vibrational effects on dissociative adsorption and associative desorption of H2Pd(100). Progress in Surface Science, 1996, 53, 187-196.	3.8	44
87	Electronic metal-support interactions and their promotional effect on CO2 methanation on Ru/ZrO2 catalysts. Journal of Catalysis, 2021, 400, 407-420.	3.1	44
88	Six-dimensional quantum dynamics of adsorption and desorption of H2 at Pd(100): no need for a molecular precursor adsorption state. Surface Science, 1996, 357-358, 614-618.	0.8	43
89	Scattering of hydrogen molecules from a reactive surface: Strong off-specular and rotationally inelastic diffraction. Chemical Physics Letters, 1996, 263, 567-573.	1.2	43
90	Improved DFT Adsorption Energies with Semiempirical Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 3250-3259.	2.3	43

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91	Sulfate, Bisulfate, and Hydrogen Co-adsorption on Pt(111) and Au(111) in an Electrochemical Environment. Frontiers in Chemistry, 2020, 8, 634.	1.8	43
92	Ab initiocalculation of the potential energy surface for the dissociation ofH2on the sulfur-covered Pd(100) surface. Physical Review B, 1998, 57, 15572-15584.	1.1	42
93	Structureâ€“reactivity relationship for bimetallic electrodes: Pt overlayers and PtAu surface alloys on Au(111). Journal of Electroanalytical Chemistry, 2007, 607, 47-53.	1.9	41
94	Interaction of Dioxygen with Al Clusters and Al(111):â€‰ A Comparative Theoretical Study. Journal of Physical Chemistry C, 2008, 112, 6924-6932.	1.5	41
95	Structural and electronic properties of oligo- and polythiophenes modified by substituents. Beilstein Journal of Nanotechnology, 2012, 3, 909-919.	1.5	39
96	Vibrational and rotational population distribution ofD2associatively desorbing from Pd(100). Physical Review B, 2001, 63, .	1.1	38
97	Hierarchically Selfâ€Assembled Hostâ€“Guest Network at the Solidâ€“Liquid Interface for Singleâ€Molecule Manipulation. Angewandte Chemie - International Edition, 2008, 47, 3821-3825.	7.2	37
98	Design of Nickel-Based Cation-Disordered Rock-Salt Oxides: The Effect of Transition Metal (M = V, Ti,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Materials & Interfaces, 2018, 10, 21957-21964.	4.0	37
99	Ab InitioBased Tight-Binding Hamiltonian for the Dissociation of Molecules at Surfaces. Physical Review Letters, 1999, 82, 1209-1212.	2.9	36
100	Kinetic Monte Carlo simulations of the interaction of oxygen with Pt(111). Journal of Chemical Physics, 2007, 127, 014704.	1.2	36
101	Intermolecular vs moleculeâ€“substrate interactions: A combined STM and theoretical study of supramolecular phases on graphene/Ru(0001). Beilstein Journal of Nanotechnology, 2011, 2, 365-373.	1.5	36
102	Coverage effects in the adsorption of H2 on Pd(100) studied by ab initio molecular dynamics simulations. Journal of Chemical Physics, 2011, 135, 174707.	1.2	35
103	Electrode/Electrolyte Interface in the Liâ€“O₂ Battery: Insight from Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 14463-14469.	1.5	34
104	Does Involving Additional Linker Always Increase the Efficiency of an Organic Dye for p-Type Dye-Sensitized Solar Cells?. ACS Applied Energy Materials, 2019, 2, 6341-6347.	2.5	33
105	Grand-canonical approaches to understand structures and processes at electrochemical interfaces from an atomistic perspective. Current Opinion in Electrochemistry, 2021, 27, 100684.	2.5	33
106	Gross and Scheffler Reply:. Physical Review Letters, 1996, 77, 405-405.	2.9	32
107	Rotational effects in the dissociation of H2 on metal surfaces studied by ab initio quantum-dynamics calculations. Chemical Physics Letters, 1999, 311, 1-7.	1.2	32
108	Dynamics of hydrogen dissociation at the sulfur-covered Pd(100) surface. Physical Review B, 2000, 61, 8425-8432.	1.1	32

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109	Kinetic Monte Carlo simulations of the partial oxidation of methanol on oxygen-covered Cu(110). Surface Science, 2006, 600, 3258-3265.	0.8	32
110	Density fluctuations as door-opener for diffusion on crowded surfaces. Science, 2019, 363, 715-718.	6.0	32
111	Surface configuration and wettability of nickel(oxy)hydroxides: a first-principles investigation. Physical Chemistry Chemical Physics, 2017, 19, 22659-22669.	1.3	31
112	Introducing Highly Redoxâ€Active Atomic Centers into Insertionâ€Type Electrodes for Lithiumâ€Ion Batteries. Advanced Energy Materials, 2020, 10, 2000783.	10.2	30
113	Vibrational excitation of NO in NO/Ag scattering revisited. Surface Science, 1993, 289, 335-339.	0.8	29
114	Ab initio based tight-binding molecular dynamics simulation of the sticking and scattering of O2â•Pt(111). Journal of Chemical Physics, 2006, 124, 174713.	1.2	29
115	Bis(terpyridine)-based surface template structures on graphite: a force field and DFT study. Physical Chemistry Chemical Physics, 2009, 11, 8867.	1.3	29
116	Polymorphism of Water in Two Dimensions. Journal of Physical Chemistry C, 2016, 120, 13649-13655.	1.5	29
117	A Molecular Double Decker: Extending the Limits of Current Metalâ€“Molecule Hybrid Structures. Angewandte Chemie - International Edition, 2010, 49, 341-345.	7.2	28
118	Hydrogen on metal surfaces: Forever young. Surface Science, 2012, 606, 690-691.	0.8	28
119	Surface temperature effects in dissociative adsorption: D2/Cu(111). Surface Science, 1994, 314, L843-L848.	0.8	27
120	CO and hydrogen adsorption on Pd(210). Surface Science, 2004, 570, 227-236.	0.8	27
121	Chemical Interactions at Metal/Molecule Interfaces in Molecular Junctionsâ€”A Pathway Towards Molecular Recognition. Advanced Materials, 2009, 21, 320-324.	11.1	27
122	Solvated protons in density functional theoryâ€”A few examples. Electrochimica Acta, 2013, 105, 248-253.	2.6	27
123	Alkali metal insertion into hard carbon â€“ the full picture. Journal of Materials Chemistry A, 2020, 8, 14205-14213.	5.2	27
124	Quantum effects in the dissociative adsorption of hydrogen. Journal of Chemical Physics, 1999, 110, 8696-8702.	1.2	26
125	Adsorption dynamics of H2 on Pd(100) from first principles. Physical Chemistry Chemical Physics, 2009, 11, 5814.	1.3	26
126	Molecular dynamics study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> on H-covered Pd(100). Physical Review B, 2010, 81, .	1.1	26

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127	Methanol Oxidation on Pt(111) from First-Principles in Heterogeneous and Electrocatalysis. Electrocatalysis, 2017, 8, 577-586.	1.5	26
128	Effect of Electron-Withdrawing/-Donating Groups on the Sensitizing Action of the Novel Organic Dye â€œ3-(5-(4-(Diphenylamino)styryl)thiophen-2-yl)-2-cyanoacrylic Acidâ€•for N-Type Dye-Sensitized Solar Cells: A Theoretical Study. Journal of Physical Chemistry C, 2020, 124, 8526-8540.	1.5	26
129	Stability, composition and properties of Li2FeSiO4 surfaces studied by DFT. Journal of Solid State Electrochemistry, 2014, 18, 1401-1413.	1.2	25
130	Local reactivity of ultrathin platinum overlayers and surface alloys on a gold surface. Surface Science, 2007, 601, 3702-3706.	0.8	23
131	Adsorption of CO on Ni/Cu(110) bimetallic surfaces. Physical Review B, 2009, 80, .	1.1	23
132	A highly ordered, aromatic bidentate self-assembled monolayer on Au(111): a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2010, 12, 6445.	1.3	23
133	Exchange processes in the contact formation of Pb electrodes. Electrochimica Acta, 2014, 140, 505-510.	2.6	23
134	Ab initio molecular dynamics simulations of the O2/Pt(1 1 1) interaction. Catalysis Today, 2016, 260, 60-65.	2.2	23
135	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	1.9	23
136	Partial oxidation of methanol on Cu(110): Energetics and kinetics. Computational and Theoretical Chemistry, 2006, 771, 117-122.	1.5	22
137	Energetics driving the short-range order in CuxPd1â€“x/Ru(0001) monolayer surface alloys. Physical Chemistry Chemical Physics, 2007, 9, 5127.	1.3	22
138	Numerically stable solution of coupled channel equations: The wave function. European Physical Journal B, 1995, 97, 311-317.	0.6	21
139	Simulation of laser-induced desorption of NO from NiO(100). Chemical Physics Letters, 2003, 376, 424-431.	1.2	21
140	High-dimensional quantum dynamical study of the dissociation of H2 on Pd(110). Journal of Chemical Physics, 2004, 120, 5339-5346.	1.2	21
141	First-principles study of the structure of water layers on flat and stepped Pb electrodes. Beilstein Journal of Nanotechnology, 2016, 7, 533-543.	1.5	21
142	Design and Tuning of the Electrochemical Properties of Vanadium-Based Cation-Disordered Rock-Salt Oxide Positive Electrode Material for Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 39848-39858.	4.0	21
143	An Alternative Charge-Storage Mechanism for High-Performance Sodium-Ion and Potassium-Ion Anodes. ACS Energy Letters, 2021, 6, 915-924.	8.8	21
144	The Dynamic Nature of CO Adlayers on Pt(111) Electrodes. Angewandte Chemie - International Edition, 2020, 59, 6182-6186.	7.2	20

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145	Theoretical Study of the O₂ Interaction with a Tetrahedral Al₄ Cluster. Journal of Physical Chemistry A, 2010, 114, 11746-11750.	1.1	19
146	Lowering Energy Barriers in Surface Reactions through Concerted Reaction Mechanisms. ChemPhysChem, 2012, 13, 3467-3471.	1.0	19
147	The role of surface defects in large organic molecule adsorption: substrate configuration effects. Physical Chemistry Chemical Physics, 2012, 14, 10726.	1.3	19
148	Ab initio molecular dynamics study of H2 adsorption on sulfur- and chlorine-covered Pd(100). Surface Science, 2013, 608, 249-254.	0.8	19
149	Descriptor and Scaling Relations for Ion Mobility in Crystalline Solids. Jacs Au, 2022, 2, 463-471.	3.6	19
150	Adiabatic versus non-adiabatic effects in the vibrational excitation in NO/Ag scattering. Chemical Physics, 1993, 177, 497-508.	0.9	18
151	From single molecules to water networks: Dynamics of water adsorption on Pt(111). Journal of Chemical Physics, 2016, 145, 094703.	1.2	18
152	Promising sensitizers for dye sensitized solar cells: A comparison of Ru(II) with other earth's scarce and abundant metal polypyridine complexes. International Journal of Quantum Chemistry, 2019, 119, e25963.	1.0	18
153	Semiclassical treatment of charge transfer in molecule-surface scattering. Journal of Chemical Physics, 2001, 114, 6396-6403.	1.2	17
154	Semiconductorâ€“metal transition induced by nanoscale stabilization. Physical Chemistry Chemical Physics, 2015, 17, 5569-5573.	1.3	17
155	Structure formation and surface chemistry of ionic liquids on model electrode surfacesâ€”Model studies for the electrode | electrolyte interface in Li-ion batteries. Journal of Chemical Physics, 2018, 148, 193821.	1.2	17
156	Fundamental Challenges for Modeling Electrochemical Energy Storage Systems at the Atomic Scale. Topics in Current Chemistry, 2018, 376, 17.	3.0	16
157	Influence of electric fields on metal self-diffusion barriers and its consequences on dendrite growth in batteries. Journal of Chemical Physics, 2019, 151, 234707.	1.2	16
158	Real-space method for total-energy calculations in semiconductors: Estimationx of stacking fault energies. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1991, 64, 413-424.	0.6	15
159	Adsorptionâ€“Desorption of H2/Si: A 5-D Dynamical Model. Physica Status Solidi A, 1997, 159, 75-90.	1.7	15
160	A systematic DFT study of substrate reconstruction effects due to thiolate and selenolate adsorption. Surface Science, 2015, 640, 18-24.	0.8	15
161	Structure Formation and Thermal Stability of Mono- and Multilayers of Ethylene Carbonate on Cu(111): A Model Study of the Electrode|Electrolyte Interface. Journal of Physical Chemistry C, 2016, 120, 16791-16803.	1.5	15
162	O2 Adsorption Dynamics at Metal Surfaces: Non-adiabatic Effects, Dissociation and Dissipation. Springer Series in Surface Sciences, 2013, , 389-419.	0.3	15

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163	Simulation of bonding effects in HRTEM images of light element materials. Beilstein Journal of Nanotechnology, 2011, 2, 394-404.	1.5	14
164	Ionic Adsorbate Structures on Metal Electrodes Calculated from First-Principles. Industrial & Engineering Chemistry Research, 2016, 55, 11107-11113.	1.8	14
165	Experimental and Computational Study on the Interaction of an Ionic Liquid Monolayer with Lithium on Pristine and Lithiated Graphite. Journal of Physical Chemistry C, 2018, 122, 18968-18981.	1.5	14
166	In Search of the Active Sites for the Selective Catalytic Reduction on Tungsten-Doped Vanadia Monolayer Catalysts Supported by TiO₂. ACS Catalysis, 2021, 11, 7411-7421.	5.5	14
167	Rotational quantum dynamics in a non-activated adsorption system. Physical Chemistry Chemical Physics, 2002, 4, 4126-4132.	1.3	13
168	Molecularâ€Scale Imaging of Water Near Charged Surfaces. ChemElectroChem, 2014, 1, 431-435.	1.7	13
169	Screening of Charge Carrier Migration in the MgSc2Se4 Spinel Structure. Frontiers in Energy Research, 2020, 8, .	1.2	13
170	On stability and kinetics of Li-rich transition metal oxides and oxyfluorides. Journal of Materials Chemistry A, 2020, 8, 7956-7967.	5.2	13
171	Reversible vs Standard Hydrogen Electrode Scale in Interfacial Electrochemistry from a Theoreticianâ€™s Atomistic Point of View. Journal of Physical Chemistry C, 2022, 126, 11439-11446.	1.5	13
172	Theoretical investigation of the interaction of CH4 with Al2 and Al3 neutral and charged clusters. Journal of Chemical Physics, 2010, 132, 154701.	1.2	12
173	Adsorption of Supramolecular Building Blocks on Graphite: A Force Field and Density Functional Theory Study. ChemPhysChem, 2011, 12, 2242-2245.	1.0	12
174	Oxidation of an Organic Adlayer: A Birdâ€™s Eye View. Journal of the American Chemical Society, 2012, 134, 8817-8822.	6.6	12
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