Axel Gross

List of Publications by Citations

242 papers	10,036 citations	59 h-index	90 g-index
281 ext. papers	11,041 ext. citations	6 avg, IF	6.99 L-index

#	Paper	IF	Citations
242	Six-dimensional quantum dynamics of adsorption and desorption of H2 at Pd(100): Steering and steric effects. *Physical Review Letters*, **1995**, 75, 2718-2721	7.4	338
241	Reactions at surfaces studied by ab initio dynamics calculations. *Surface Science Reports*, **1998**, 32, 291-340	12.9	323
240	Surface strain versus substrate interaction in heteroepitaxial metal layers: Pt on Ru(0001). *Physical Review Letters*, **2003**, 91, 016101	7.4	282
239	Representing high-dimensional potential-energy surfaces for reactions at surfaces by neural networks. *Chemical Physics Letters*, **2004**, 395, 210-215	2.5	262
238	Properties of metal water interfaces studied from first principles. *New Journal of Physics*, **2009**, 11, 125003	3.9	239
237	Experimental analysis of charge redistribution due to chemical bonding by high-resolution transmission electron microscopy. *Nature Materials*, **2011**, 10, 209-15	27	237
236	Microscopic properties of lithium, sodium, and magnesium battery anode materials related to possible dendrite growth. *Journal of Chemical Physics*, **2014**, 141, 174710	3.9	207
235	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	3.9	201
234	Reactivity of Bimetallic Systems Studied from First Principles. *Topics in Catalysis*, **2006**, 37, 29-39	2.3	174
233	Quantum theory of dissociative chemisorption on metal surfaces. *Accounts of Chemical Research*, **2002**, 35, 193-200	24.3	154
232	Ab initio quantum and molecular dynamics of the dissociative adsorption of hydrogen on Pd(100). *Physical Review B*, **1998**, 57, 2493-2506	3.3	148
231	Self-diffusion barriers: possible descriptors for dendrite growth in batteries?. *Energy and Environmental Science*, **2018**, 11, 3400-3407	35.4	144
230	Toward an Atomic-Scale Understanding of Electrochemical Interface Structure and Dynamics. *Journal of the American Chemical Society*, **2019**, 141, 4777-4790	16.4	139
229	Fluoride ion batteries: Theoretical performance, safety, toxicity, and a combinatorial screening of new electrodes. *Journal of Fluorine Chemistry*, **2016**, 182, 76-90	2.1	136
228	High-dimensional quantum dynamics of adsorption and desorption of H2 at Cu(111). *Physical Review Letters*, **1994**, 73, 3121-3124	7.4	131
227	Challenges in the first-principles description of reactions in electrocatalysis. *Catalysis Today*, **2011**, 165, 129-137	5.3	128
226	Dissociative adsorption of hydrogen on strained Cu surfaces. *Surface Science*, **2003**, 525, 107-118	1.8	128

225	Local reactivity of thin Pd overlayers on Au single crystals. *Journal of Electroanalytical Chemistry*, **2003**, 548, 121-130	4.1	125
224	Local reactivity of metal overlayers: Density functional theory calculations of Pd on Au. *Physical Review B*, **2003**, 67,	3.3	123
223	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	3.5	119
222	Descriptions of surface chemical reactions using a neural network representation of the potential-energy surface. *Physical Review B*, **2006**, 73,	3.3	103
221	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	3.9	101
220	Hydrogen dissociation dynamics on precovered Pd surfaces: Langmuir is still right. *Physical Review Letters*, **2007**, 98, 206107	7.4	100
219	Water bilayer on the Pd/Au(111) overlayer system: Coadsorption and electric field effects. *Chemical Physics Letters*, **2005**, 409, 157-162	2.5	100
218	The Importance of the Electrochemical Environment in the Electro-Oxidation of Methanol on Pt(111). *ACS Catalysis*, **2016**, 6, 5575-5586	13.1	97
217	Density functional theory study of the partial oxidation of methanol on copper surfaces. *Journal of Catalysis*, **2005**, 231, 420-429	7.3	97
216	Numerically stable solution of coupled channel equations: The local reflection matrix. *European Physical Journal B*, **1993**, 93, 91-101	1.2	94
215	Local density of states effects at the metal-molecule interfaces in a molecular device. *Nature Materials*, **2006**, 5, 394-9	27	93
214	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	3.9	92
213	Dispersion corrected RPBE studies of liquid water. *Journal of Chemical Physics*, **2014**, 141, 064501	3.9	90
212	Insight into Sodium Insertion and the Storage Mechanism in Hard Carbon. *ACS Energy Letters*, **2018**, 3, 2851-2857	20.1	89
211	The electric double layer at metal-water interfaces revisited based on a charge polarization scheme. *Journal of Chemical Physics*, **2018**, 149, 084705	3.9	87
210	Strain and coordination effects in the adsorption properties of early transition metals: A density-functional theory study. *Physical Review B*, **2010**, 81,	3.3	87
209	Tuning catalytic properties of bimetallic surfaces: Oxygen adsorption on pseudomorphic Pt/Ru overlayers. *Electrochimica Acta*, **2007**, 52, 2219-2228	6.7	85
208	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, 7773-84	16.7	84

207	Theoretical Surface Science **2009**,		84
206	Change of the work function of platinum electrodes induced by halide adsorption. *Beilstein Journal of Nanotechnology*, **2014**, 5, 152-61	3	79
205	The role of lateral surface corrugation for the quantum dynamics of dissociative adsorption and associative desorption. *Journal of Chemical Physics*, **1995**, 102, 5045-5058	3.9	77
204	Structure of water layers on hydrogen-covered Pt electrodes. *Catalysis Today*, **2013**, 202, 183-190	5.3	74
203	Concentration and Coverage Dependent Adlayer Structures: From Two-Dimensional Networks to Rotation in a Bearing. *Journal of Physical Chemistry C*, **2010**, 114, 1268-1277	3.8	74
202	CO adsorption on Cu-Pd alloy surfaces: ligand versus ensemble effects. *Physical Chemistry Chemical Physics*, **2007**, 9, 2216-25	3.6	74
201	Hydrogen adsorption on an open metal surface: H2/Pd(210). *Physical Review B*, **2002**, 65,	3.3	74
200	Reaction dynamics of molecular hydrogen on silicon surfaces. *Physical Review B*, **1996**, 54, 5978-5991	3.3	72
199	Total oxidation of methanol on Cu(110): a density functional theory study. *Journal of Physical Chemistry A*, **2007**, 111, 8814-22	2.8	70
198	Local reactivity of supported metal clusters: Pdn on Au(1 1 1). *Surface Science*, **2004**, 559, L180-L186	1.8	70
197	The virtual chemistry lab for reactions at surfaces: Is it possible? Will it be useful?. *Surface Science*, **2002**, 500, 347-367	1.8	70
196	Signatures of nonadiabatic O2 dissociation at Al(111): First-principles fewest-switches study. *Physical Review B*, **2010**, 81,	3.3	69
195	Fingerprints for spin-selection rules in the interaction dynamics of O2 at Al(111). *Physical Review Letters*, **2008**, 101, 096104	7.4	68
194	Unified picture of the molecular adsorption process: O2/Pt(111). *Surface Science*, **2003**, 539, L542-L548	1.8	68
193	Water Structures at Metal Electrodes Studied by Ab Initio Molecular Dynamics Simulations. *Journal of the Electrochemical Society*, **2014**, 161, E3015-E3020	3.9	67
192	First-principles study of the water structure on flat and stepped gold surfaces. *Surface Science*, **2012**, 606, 886-891	1.8	67
191	Periodic density-functional calculations on work-function change induced by adsorption of halogens on Cu(111). *Physical Review Letters*, **2013**, 110, 156804	7.4	67
190	Influence of water on elementary reaction steps in electrocatalysis. *Faraday Discussions*, **2008**, 140, 233-44; discussion 297-317	3.6	67

189	Ab Initio Molecular Dynamics Study of the Desorption of D2 from Si(100). *Physical Review Letters*, **1997**, 79, 701-704	7.4	65
188	Theoretical Surface Science. *Advanced Texts in Physics*, **2003**,		63
187	Trends in the chemical reactivity of surfaces studied by ab initio quantum-dynamics calculations. *Physical Review B*, **1999**, 59, 13297-13300	3.3	63
186	Equilibrium coverage of halides on metal electrodes. *Surface Science*, **2015**, 631, 17-22	1.8	62
185	Coexistence of atomic and molecular chemisorption states: H(2)/Pd(210). *Physical Review Letters*, **2001**, 87, 096103	7.4	62
184	Influence of molecular vibrations on dissociative adsorption. *Chemical Physics Letters*, **1996**, 256, 417-423	2.5	60
183	Adsorption at Nanostructured Surfaces from First Principles. *Journal of Computational and Theoretical Nanoscience*, **2008**, 5, 894-922	0.3	59
182	Operando pH Measurements Decipher H+/Zn2+ Intercalation Chemistry in High-Performance Aqueous Zn/V2O5 Batteries. *ACS Energy Letters*, **2020**, 5, 2979-2986	20.1	58
181	Modelling the electric double layer at electrode/electrolyte interfaces. *Current Opinion in Electrochemistry*, **2019**, 14, 1-6	7.2	57
180	Hierarchical interactions and their influence upon the adsorption of organic molecules on a graphene film. *Journal of the American Chemical Society*, **2011**, 133, 9208-11	16.4	55
179	Detailed balance and phonon assisted sticking in adsorption and desorption of H2/Si. *European Physical Journal B*, **1994**, 96, 231-234	1.2	53
178	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	2.9	51
177	Hydrogen and halide co-adsorption on Pt(111) in an electrochemical environment: a computational perspective. *Electrochimica Acta*, **2016**, 216, 152-159	6.7	51
176	Hydrogen adsorption energies on bimetallic overlayer systems at the solid–vacuum and the solid–liquid interface. *Surface Science*, **2005**, 597, 42-50	1.8	49
175	Interaction of a Self-Assembled Ionic Liquid Layer with Graphite(0001): A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry Letters*, **2016**, 7, 226-33	6.4	47
174	Adsorption of 4-mercaptopyridine on Au(111: a periodic DFT study. *Langmuir*, **2008**, 24, 13985-92	4	47
173	Tailoring the reactivity of bimetallic overlayer and surface alloy systems. *Journal of Physics Condensed Matter*, **2009**, 21, 084205	1.8	45
172	Hydrogen dissociation on metal surfaces—a model system for reactions on surfaces. *Applied Physics A: Materials Science and Processing*, **1998**, 67, 627-635	2.6	45

171	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	1.8	45
170	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	8.9	44
169	Ab initio molecular dynamics study of hot atom dynamics after dissociative adsorption of H2 on Pd(100). *Physical Review Letters*, **2009**, 103, 246101	7.4	44
168	Dynamical quantum processes of molecular beams at surfaces: dissociative adsorption of hydrogen on metal surfaces. *Surface Science*, **1996**, 363, 1-10	1.8	44
167	Ab initio molecular dynamics simulations of the adsorption of H2 on palladium surfaces. *ChemPhysChem*, **2010**, 11, 1374-81	3.2	43
166	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	1.8	41
165	Scattering of hydrogen molecules from a reactive surface: Strong off-specular and rotationally inelastic diffraction. *Chemical Physics Letters*, **1996**, 263, 567-573	2.5	41
164	Structure and local reactivity of PdAg/Pd(111) surface alloys. *Physical Chemistry Chemical Physics*, **2013**, 15, 1497-508	3.6	39
163	Interaction of Dioxygen with Al Clusters and Al(111): A Comparative Theoretical Study. *Journal of Physical Chemistry C*, **2008**, 112, 6924-6932	3.8	39
162	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	20.1	39
161	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	3.6	38
160	Vibrational and rotational population distribution of D2 associatively desorbing from Pd(100). *Physical Review B*, **2001**, 63,	3.3	38
159	Ab initio calculation of the potential energy surface for the dissociation of H2 on the sulfur-covered Pd(100) surface. *Physical Review B*, **1998**, 57, 15572-15584	3.3	38
158	Steering and ro-vibrational effects on dissociative adsorption and associative desorption of H2Pd(100). *Progress in Surface Science*, **1996**, 53, 187-196	6.6	38
157	Halide adsorption on close-packed metal electrodes. *Physical Chemistry Chemical Physics*, **2014**, 16, 13630-4	3.4	37
156	Structure–reactivity relationship for bimetallic electrodes: Pt overlayers and PtAu surface alloys on Au(111). *Journal of Electroanalytical Chemistry*, **2007**, 607, 47-53	4.1	36
155	Hierarchically self-assembled host-guest network at the solid-liquid interface for single-molecule manipulation. *Angewandte Chemie - International Edition*, **2008**, 47, 3821-5	16.4	36
154	Ab Initio Based Tight-Binding Hamiltonian for the Dissociation of Molecules at Surfaces. *Physical Review Letters*, **1999**, 82, 1209-1212	7.4	35

153	Structural and electronic properties of oligo- and polythiophenes modified by substituents. *Beilstein Journal of Nanotechnology*, **2012**, 3, 909-19	3	34
152	Intermolecular vs molecule-substrate interactions: A combined STM and theoretical study of supramolecular phases on graphene/Ru(0001). *Beilstein Journal of Nanotechnology*, **2011**, 2, 365-73	3	34
151	Insights into the electrochemical processes of rechargeable magnesium–sulfur batteries with a new cathode design. *Journal of Materials Chemistry A*, **2019**, 7, 25490-25502	13	33
150	Coverage effects in the adsorption of H2 on Pd(100) studied by ab initio molecular dynamics simulations. *Journal of Chemical Physics*, **2011**, 135, 174707	3.9	32
149	Dynamics of hydrogen dissociation at the sulfur-covered Pd(100) surface. *Physical Review B*, **2000**, 61, 8425-8432	3.3	32
148	Rotational effects in the dissociation of H2 on metal surfaces studied by ab initio quantum-dynamics calculations. *Chemical Physics Letters*, **1999**, 311, 1-7	2.5	32
147	Kinetic Monte Carlo simulations of the interaction of oxygen with Pt(111). *Journal of Chemical Physics*, **2007**, 127, 014704	3.9	31
146	Kinetic Monte Carlo simulations of the partial oxidation of methanol on oxygen-covered Cu(110). *Surface Science*, **2006**, 600, 3258-3265	1.8	30
145	Gross and Scheffler Reply. *Physical Review Letters*, **1996**, 77, 405	7.4	30
144	Improved DFT Adsorption Energies with Semiempirical Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2019**, 15, 3250-3259	6.4	29
143	Ab initio based tight-binding molecular dynamics simulation of the sticking and scattering of O2Pt(111). *Journal of Chemical Physics*, **2006**, 124, 174713	3.9	29
142	Vibrational excitation of NO in NO/Ag scattering revisited. *Surface Science*, **1993**, 289, 335-339	1.8	29
141	Bis(terpyridine)-based surface template structures on graphite: a force field and DFT study. *Physical Chemistry Chemical Physics*, **2009**, 11, 8867-78	3.6	28
140	Hydrogen on metal surfaces: Forever young. *Surface Science*, **2012**, 606, 690-691	1.8	27
139	Sulfate, Bisulfate, and Hydrogen Co-adsorption on Pt(111) and Au(111) in an Electrochemical Environment. *Frontiers in Chemistry*, **2020**, 8, 634	5	27
138	Electrode/Electrolyte Interface in the Li–O2 Battery: Insight from Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2017**, 121, 14463-14469	3.8	26
137	Chemical Interactions at Metal/Molecule Interfaces in Molecular Junctions—A Pathway Towards Molecular Recognition. *Advanced Materials*, **2009**, 21, 320-324	24	26
136	A molecular double decker: extending the limits of current metal-molecule hybrid structures. *Angewandte Chemie - International Edition*, **2010**, 49, 341-5	16.4	26

135	Polymorphism of Water in Two Dimensions. *Journal of Physical Chemistry C*, **2016**, 120, 13649-13655	3.8	25
134	Design of Nickel-Based Cation-Disordered Rock-Salt Oxides: The Effect of Transition Metal (M = V, Ti, Zr) Substitution in LiNiMO Binary Systems. *ACS Applied Materials & Interfaces*, **2018**, 10, 21957-21964	9.5	25
133	Adsorption dynamics of H2 on Pd(100) from first principles. *Physical Chemistry Chemical Physics*, **2009**, 11, 5814-22	3.6	25
132	Quantum effects in the dissociative adsorption of hydrogen. *Journal of Chemical Physics*, **1999**, 110, 8696-8702	3.9	25
131	Surface temperature effects in dissociative adsorption: D2/Cu(111). *Surface Science*, **1994**, 314, L843-L848	1.8	25
130	Density fluctuations as door-opener for diffusion on crowded surfaces. *Science*, **2019**, 363, 715-718	33.3	25
129	Stability, composition and properties of Li2FeSiO4 surfaces studied by DFT. *Journal of Solid State Electrochemistry*, **2014**, 18, 1401-1413	2.6	24
128	CO and hydrogen adsorption on Pd(2 1 0). *Surface Science*, **2004**, 570, 227-236	1.8	24
127	Ab initio molecular dynamics simulations of the O2/Pt(1 1 1) interaction. *Catalysis Today*, **2016**, 260, 60-65	5.3	23
126	Surface configuration and wettability of nickel(oxy)hydroxides: a first-principles investigation. *Physical Chemistry Chemical Physics*, **2017**, 19, 22659-22669	3.6	23
125	Solvated protons in density functional theory: A few examples. *Electrochimica Acta*, **2013**, 105, 248-253	6.7	23
124	Molecular dynamics study of H2 dissociation on H-covered Pd(100). *Physical Review B*, **2010**, 81,	3.3	23
123	Adsorption of CO on Ni/Cu(110) bimetallic surfaces. *Physical Review B*, **2009**, 80,	3.3	23
122	Energetics driving the short-range order in CuxPd1-x/Ru(0001) monolayer surface alloys. *Physical Chemistry Chemical Physics*, **2007**, 9, 5127-32	3.6	22
121	Local reactivity of ultrathin platinum overlayers and surface alloys on a gold surface. *Surface Science*, **2007**, 601, 3702-3706	1.8	21
120	Simulation of laser-induced desorption of NO from NiO(100). *Chemical Physics Letters*, **2003**, 376, 424-431	2.5	21
119	Numerically stable solution of coupled channel equations: The wave function. *European Physical Journal B*, **1995**, 97, 311-317	1.2	21
118	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	13	21

117	Methanol Oxidation on Pt(111) from First-Principles in Heterogeneous and Electrocatalysis. *Electrocatalysis*, **2017**, 8, 577-586	2.7	20
116	Introducing Highly Redox-Active Atomic Centers into Insertion-Type Electrodes for Lithium-Ion Batteries. *Advanced Energy Materials*, **2020**, 10, 2000783	21.8	20
115	High-dimensional quantum dynamical study of the dissociation of H2 on Pd110. *Journal of Chemical Physics*, **2004**, 120, 5339-46	3.9	20
114	Exchange processes in the contact formation of Pb electrodes. *Electrochimica Acta*, **2014**, 140, 505-510	6.7	19
113	A highly ordered, aromatic bidentate self-assembled monolayer on Au(111): a combined experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2010**, 12, 6445-54	3.6	19
112	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	6.1	18
111	Ab initio molecular dynamics study of H2 adsorption on sulfur- and chlorine-covered Pd(100). *Surface Science*, **2013**, 608, 249-254	1.8	18
110	Partial oxidation of methanol on Cu(110): Energetics and kinetics. *Computational and Theoretical Chemistry*, **2006**, 771, 117-122		18
109	Grand-canonical approaches to understand structures and processes at electrochemical interfaces from an atomistic perspective. *Current Opinion in Electrochemistry*, **2021**, 27, 100684	7.2	18
108	Lowering energy barriers in surface reactions through concerted reaction mechanisms. *ChemPhysChem*, **2012**, 13, 3467-71	3.2	17
107	Theoretical study of the O□nteraction with a tetrahedral Al□cluster. *Journal of Physical Chemistry A* , **2010**, 114, 11746-50	2.8	17
106	Semiclassical treatment of charge transfer in molecule-surface scattering. *Journal of Chemical Physics*, **2001**, 114, 6396-6403	3.9	17
105	Adiabatic versus non-adiabatic effects in the vibrational excitation in NO/Ag scattering. *Chemical Physics*, **1993**, 177, 497-508	2.3	17
104	First-principles study of the structure of water layers on flat and stepped Pb electrodes. *Beilstein Journal of Nanotechnology*, **2016**, 7, 533-43	3	17
103	The role of surface defects in large organic molecule adsorption: substrate configuration effects. *Physical Chemistry Chemical Physics*, **2012**, 14, 10726-31	3.6	16
102	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	9.5	15
101	From single molecules to water networks: Dynamics of water adsorption on Pt(111). *Journal of Chemical Physics*, **2016**, 145, 094703	3.9	15
100	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		14

99	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	3.8	14
98	Semiconductor-metal transition induced by nanoscale stabilization. *Physical Chemistry Chemical Physics*, **2015**, 17, 5569-73	3.6	13
97	Structure formation and surface chemistry of ionic liquids on model electrode surfaces-Model studies for the electrode electrolyte interface in Li-ion batteries. *Journal of Chemical Physics*, **2018**, 148, 193821	3.9	13
96	Simulation of bonding effects in HRTEM images of light element materials. *Beilstein Journal of Nanotechnology*, **2011**, 2, 394-404	3	13
95	Rotational quantum dynamics in a non-activated adsorption system. *Physical Chemistry Chemical Physics*, **2002**, 4, 4126-4132	3.6	13
94	The Dynamic Nature of CO Adlayers on Pt(111) Electrodes. *Angewandte Chemie - International Edition*, **2020**, 59, 6182-6186	16.4	13
93	A systematic DFT study of substrate reconstruction effects due to thiolate and selenolate adsorption. *Surface Science*, **2015**, 640, 18-24	1.8	12
92	Theory of Solid/Electrolyte Interfaces **2020**, 471-515		12
91	Adsorption of supramolecular building blocks on graphite: a force field and density functional theory study. *ChemPhysChem*, **2011**, 12, 2242-5	3.2	12
90	Adsorption□Desorption of H2/Si: A 5-D Dynamical Model. *Physica Status Solidi A*, **1997**, 159, 75-90		12
89	Ein hierarchisch selbstorganisiertes Wirt-Gast-Netzwerk an der Fest-flüssig-Grenzfläche für die Manipulation einzelner Moleküle. *Angewandte Chemie*, **2008**, 120, 3881-3885	3.6	12
88	O2 Adsorption Dynamics at Metal Surfaces: Non-adiabatic Effects, Dissociation and Dissipation. *Springer Series in Surface Sciences*, **2013**, 389-419	0.4	12
87	Effect of Electron-Withdrawing/-Donating Groups on the Sensitizing Action of the Novel Organic Dye □-(5-(4-(Diphenylamino)styryl)thiophen-2-yl)-2-cyanoacrylic Acid□for N-Type Dye-Sensitized Solar Cells: A Theoretical Study. *Journal of Physical Chemistry C*, **2020**, 124, 8526-8540	3.8	11
86	Alkali metal insertion into hard carbon□the full picture. *Journal of Materials Chemistry A*, **2020**, 8, 14205-14213	13	11
85	Polar surface energies of iono-covalent materials: implications of a charge-transfer model tested on Li2FeSiO4 surfaces. *ChemPhysChem*, **2014**, 15, 2058-69	3.2	11
84	Molecular-Scale Imaging of Water Near Charged Surfaces. *ChemElectroChem*, **2014**, 1, 431-435	4.3	11
83	Influence of the solvent on the stability of bis(terpyridine) structures on graphite. *Beilstein Journal of Nanotechnology*, **2013**, 4, 269-77	3	11
82	Theoretical investigation of the interaction of CH(4) with Al(2) and Al(3) neutral and charged clusters. *Journal of Chemical Physics*, **2010**, 132, 154701	3.9	11

81	Rotational and vibrational population of D2 desorbing from sulfur-covered Pd(100). *Physical Review B*, **2002**, 66,	3.3	11
80	Ab Initio Simulations of Water/Metal Interfaces.. *Chemical Reviews*, **2022**,	68.1	11
79	Ionic Adsorbate Structures on Metal Electrodes Calculated from First-Principles. *Industrial & Engineering Chemistry Research*, **2016**, 55, 11107-11113	3.9	11
78	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	2.1	10
77	Fundamental Challenges for Modeling Electrochemical Energy Storage Systems at the Atomic Scale. *Topics in Current Chemistry*, **2018**, 376, 17	7.2	10
76	Adsorption of Ultrathin Ethylene Carbonate Films on Pristine and Lithiated Graphite and Their Interaction with Li. *Langmuir*, **2018**, 34, 8451-8463	4	10
75	Geometric and electronic structure of Pd/4-aminothiophenol/Au(111) metal-molecule-metal contacts: a periodic DFT study. *Physical Chemistry Chemical Physics*, **2010**, 12, 4423-30	3.6	10
74	Water adsorption on bimetallic PtRu/Pt(111) surface alloys. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2016**, 472, 20160618	2.4	10
73	Influence of electric fields on metal self-diffusion barriers and its consequences on dendrite growth in batteries. *Journal of Chemical Physics*, **2019**, 151, 234707	3.9	10
72	An Alternative Charge-Storage Mechanism for High-Performance Sodium-Ion and Potassium-Ion Anodes. *ACS Energy Letters*, **2021**, 6, 915-924	20.1	10
71	On stability and kinetics of Li-rich transition metal oxides and oxyfluorides. *Journal of Materials Chemistry A*, **2020**, 8, 7956-7967	13	9
70	Interaction of CO with PtxAg1-x/Pt(111) surface alloys: More than dilution by Ag atoms. *Surface Science*, **2016**, 650, 237-254	1.8	9
69	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	3.8	9
68	Bottom-up formation of robust gold carbide. *Scientific Reports*, **2015**, 5, 8891	4.9	9
67	Oxidation of an organic adlayer: a bird's eye view. *Journal of the American Chemical Society*, **2012**, 134, 8817-22	16.4	9
66	4,4?-Dithiodipyridine on Au(111): A Combined STM, STS, and DFT Study. *Journal of Physical Chemistry C*, **2013**, 117, 20060-20067	3.8	9
65	Quantum dynamics of the dissociation of H2 on Rh(111). *European Physical Journal B*, **2005**, 45, 425-432	1.2	9
64	Semiclassical treatment of reactions at surfaces with electronic transitions. *Faraday Discussions*, **2000**, 99-108; discussion 161-89	3.6	9

63	Influence of Step and Island Edges on Local Adsorption Properties: Hydrogen Adsorption on Pt Monolayer Island Modified Ru(0001) Electrodes. *Electrocatalysis*, **2017**, 8, 530-539	2.7	8
62	Stabilization of the Sn phase in tin nanoparticles and nanowires. *Applied Physics Letters*, **2015**, 107, 123101	3.4	8
61	Reduced Pd density of states in Pd/SAM/Au junctions: the role of adsorbed hydrogen atoms. *Physical Chemistry Chemical Physics*, **2012**, 14, 2353-61	3.6	8
60	Vibrational excitation in the scattering from an almost rigid surface: NO/diamond(110). *Surface Science*, **1994**, 302, 403-409	1.8	8
59	Diffusion on a Crowded Surface: kMC Simulations. *Journal of Physical Chemistry C*, **2020**, 124, 15216-15224	3.8	7
58	Ab initio investigation of the laser induced desorption of iodine from KI(100). *Applied Physics A: Materials Science and Processing*, **2007**, 88, 579-586	2.6	7
57	Multiplicity of atomic reconfigurations in an electrochemical Pb single-atom transistor. *Physical Review B*, **2017**, 95,	3.3	6
56	Influence of Local Inhomogeneities and the Electrochemical Environment on the Oxygen Reduction Reaction on Pt-Based Electrodes: A DFT Study. *Journal of Physical Chemistry C*, **2020**, 124, 27604-27613	3.8	6
55	Strain Dependence of Metal Anode Surface Properties. *ChemSusChem*, **2020**, 13, 3147-3153	8.3	6
54	Spiral adsorbate structures on monoatomic nanowire electrodes. *ChemPhysChem*, **2008**, 9, 1371-4	3.2	6
53	Ab initio Molecular Dynamics Simulations of Reactions at Surfaces. *Physica Status Solidi (B): Basic Research*, **2000**, 217, 389-404	1.3	6
52	Phase field parameters for battery compounds from first-principles calculations. *Physical Review Materials*, **2019**, 3,	3.2	6
51	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	13.1	6
50	Vacancy assisted diffusion on single-atom surface alloys. *ChemPhysChem*, **2021**, 22, 29-39	3.2	6
49	Model Studies on the Formation of the Solid Electrolyte Interphase: Reaction of Li with Ultrathin Adsorbed Ionic-Liquid Films and Co O (111) Thin Films. *ChemPhysChem*, **2021**, 22, 441-454	3.2	6
48	Reaction energetics of hydrogen on Si(100) surface: A periodic many-electron theory study. *Journal of Chemical Physics*, **2018**, 149, 244105	3.9	6
47	Electronic metal-support interactions and their promotional effect on CO2 methanation on Ru/ZrO2 catalysts. *Journal of Catalysis*, **2021**, 400, 407-420	7.3	6
46	Cation Overcrowding Effect on the Oxygen Evolution Reaction. *Jacs Au*, **2021**, 1, 1752-1765		6

45	FAIR data enabling new horizons for materials research.. *Nature*, **2022**, 604, 635-642	50.4	6
44	Interaction between Li, Ultrathin Adsorbed Ionic Liquid Films, and CoO(111) Thin Films: A Model Study of the Solid|Electrolyte Interphase Formation. *Chemistry of Materials*, **2019**, 31, 5537-5549	9.6	5
43	Temperature effects in the vibrational spectra of self-assembled monolayers. *Physical Review Letters*, **2013**, 111, 086102	7.4	5
42	Septipyridines as conformationally controlled substitutes for inaccessible bis(terpyridine)-derived oligopyridines in two-dimensional self-assembly. *Beilstein Journal of Nanotechnology*, **2011**, 2, 405-15	3	5
41	Quantum electron transport through ultrathin Si films: effects of interface passivation on Fermi-level pinning. *Physical Review Letters*, **2008**, 101, 166801	7.4	5
40	Dynamics of molecule-surface interactions from first principles. *Chemical Physics of Solid Surfaces*, **2003**, 11, 1-26		5
39	Impact of Cathodic Electric Double Layer Composition on the Performance of Aprotic Li-O2 Batteries. *Journal of the Electrochemical Society*, **2021**, 168, 030520	3.9	5
38	Predicting Accurate Phonon Spectra: An Improved Description of Lattice Dynamics in Thermoelectric Clathrates Based on the SCAN Meta-GGA Functional. *Chemistry of Materials*, **2019**, 31, 2571-2576	9.6	4
37	Screening of Charge Carrier Migration in the MgSc2Se4 Spinel Structure. *Frontiers in Energy Research*, **2020**, 8,	3.8	4
36	Ab Initio Transport Calculations for Single-Atom Copper Junctions in the Presence of Hydrogen Chloride. *Journal of Physical Chemistry C*, **2014**, 118, 28252-28257	3.8	4
35	Theoretical Study of the O2 + Al4 (Tetrahedral) System in Its Singlet State and Comparisons with Its Triplet State. *Journal of Physical Chemistry C*, **2012**, 116, 16430-16435	3.8	4
34	Influence of water on the properties of an Au/Mpy/Pd metal/molecule/metal junction. *Beilstein Journal of Nanotechnology*, **2011**, 2, 384-93	3	4
33	Cyanophenyl vs. pyridine substituent: impact on the adlayer structure and formation on HOPG and Au(111). *Physical Chemistry Chemical Physics*, **2016**, 18, 6668-75	3.6	3
32	Challenges in bimetallic multilayer structure formation: Pt growth on Cu monolayers on Ru(0001). *Physical Chemistry Chemical Physics*, **2017**, 19, 24100-24114	3.6	3
31	Dynamics of Reactions at Surfaces **2011**, 39-70		3
30	Monodisperse microisland formation on Ni/Ru(0001) monolayers. *Physical Review Letters*, **2008**, 101, 206101	7.4	3
29	Quantum Theory of Reactive Scattering and Adsorption at Surfaces **2005**, 1713-1733		3
28	The Structure of the Electric Double Layer: Atomistic vs. Continuum Approaches. *Current Opinion in Electrochemistry*, **2022**, 100953	7.2	2

27	On the first step in zinc deposition – A case of nonlinear coupling with the solvent. *Electrochemistry Communications*, **2021**, 122, 106876	5.1	2
26	Mechanism of Magnesium Transport in Spinel Chalcogenides. *Advanced Energy and Sustainability Research*,2100113	1.6	2
25	Reversible vs Standard Hydrogen Electrode Scale in Interfacial Electrochemistry from a Theoretician's Atomistic Point of View. *Journal of Physical Chemistry C*,	3.8	2
24	Elementary Reaction Steps in Electrocatalysis: Theory Meets Experiment. *Electrocatalysis*, **2017**, 8, 499-500	2.7	1
23	Electronic factors determining the methane bond breaking process on small aluminum clusters. *International Journal of Quantum Chemistry*, **2019**, 119, e26003	2.1	1
22	Elementary Molecule–Surface Scattering Processes Relevant to Heterogeneous Catalysis: Insights from Quantum Dynamics Calculations. *Physical Chemistry in Action*, **2014**, 31-58		1
21	Quantum delocalization and correlation effects in one-dimensional chains of adsorbed hydrogen atoms. *Physical Review B*, **2010**, 82,	3.3	1
20	Composition and Electronic Structure of Mn_3O_4 and Co_3O_4 Cathodes in Zinc–Air Batteries: A DFT Study. *Journal of Physical Chemistry C*, **2022**, 126, 2561-2572	3.8	1
19	Descriptor and Scaling Relations for Ion Mobility in Crystalline Solids.. *Jacs Au*, **2022**, 2, 463-471		1
18	Interaction of Mg with the ionic liquid 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide—An experimental and computational model study of the electrode–electrolyte interface in post-lithium batteries. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2022**, 40, 023204	2.9	1
17	Structure of PtRu/Ru(0 0 0 1) and AgPd/Pd(1 1 1) surface alloys: A kinetic Monte Carlo study. *Chemical Physics*, **2022**, 555, 111428	2.3	1
16	Fundamental Challenges for Modeling Electrochemical Energy Storage Systems at the Atomic Scale. *Topics in Current Chemistry Collections*, **2018**, 1-22	1.8	1
15	Molecular Dynamics of the Electrochemical Interface and the Double Layer **2021**, 201-220		1
14	Deprotonation and Cation Adsorption on the NiOOH/Water Interface: A Grand-Canonical First-Principles Investigation. *Electrochimica Acta*, **2021**, 139253	6.7	1
13	Lithium-Ion Batteries: Introducing Highly Redox-Active Atomic Centers into Insertion-Type Electrodes for Lithium-Ion Batteries (Adv. Energy Mater. 25/2020). *Advanced Energy Materials*, **2020**, 10, 2070112	21.8	0
12	The role of anchoring groups in ruthenium(II)-bipyridine sensitized p-type semiconductor solar cells– quantum chemical approach. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2020**, 53, 234001	1.3	0
11	Coupling of photoactive transition metal complexes to a functional polymer matrix*. *Chemistry - A European Journal*, **2021**, 27, 17104-17114	4.8	0
10	First-Principles Study of the Surfaces and Equilibrium Shape of Discharge Products in Li-Air Batteries. *ACS Applied Materials & Interfaces*, **2021**, 13, 24984-24994	9.5	0

9	Mechanism of Magnesium Transport in Spinel Chalcogenides. *Advanced Energy and Sustainability Research*, **2021**, 2, 2170032	1.6	0
8	Structure of Electrode-Electrolyte Interfaces, Modeling of Double Layer and Electrode Potential **2018**, 1-34		
7	Computational Modeling of Electrocatalytic Reactions **2018**, 455-465		
6	Surface alloying in the Sn/Ni(111) system studied by synchrotron radiation photoelectron valence band spectroscopy and ab-initio density of states calculations. *Thin Solid Films*, **2008**, 516, 2962-2965	2.2	
5	Physikalische Chemie 2001. *Nachrichten Aus Der Chemie*, **2002**, 50, 336-345	0.1	
4	Structure of Electrode-Electrolyte Interfaces, Modeling of Double Layer and Electrode Potential **2020**, 1439-1472		
3	Restructuring of Lead Electrodes upon Adsorption of NO3 Anions Studied from First-Principles and Its Relevance for the Operation of Lead Quantum Switches. *Journal of Physical Chemistry C*, **2021**, 125, 17962-17970	3.8	
2	Hot atom chemistry: Oxygen at stepped platinum surfaces. *Applied Surface Science Advances*, **2022**, 9, 100240	2.6	
1	Quantum Theory of Reactive Scattering and Adsorption at Surfaces **2005**, 1713-1733		