Martin Andersson

List of Publications by Year
in descending order

103 papers	5,736 citations	117453 34 h-index	76769 74 g-index
104 all docs	104 docs citations	104 times ranked	7032 citing authors

#	Article	IF	Citations
1	New Scale Factors for Harmonic Vibrational Frequencies Using the B3LYP Density Functional Method with the Triple-Î¶ Basis Set 6-311+G(d,p). Journal of Physical Chemistry A, 2005, 109, 2937-2941.	1.1	1,324
2	First principles calculations and experimental insight into methane steam reforming over transition metal catalysts. Journal of Catalysis, 2008, 259, 147-160.	3.1	559
3	Structure sensitivity of the methanation reaction: H2-induced CO dissociation on nickel surfaces. Journal of Catalysis, 2008, 255, 6-19.	3.1	411
4	Toward computational screening in heterogeneous catalysis: Pareto-optimal methanation catalysts. Journal of Catalysis, 2006, 239, 501-506.	3.1	314
5	CO adsorption energies on metals with correction for high coordination adsorption sites â€“ A density functional study. Surface Science, 2007, 601, 1747-1753.	0.8	259
6	Direct observation of ionic structure at solid-liquid interfaces: a deep look into the Stern Layer. Scientific Reports, 2014, 4, 4956.	1.6	160
7	HandaPhos: A General Ligand Enabling Sustainable ppm Levels of Palladiumâ€Catalyzed Crossâ€Couplings in Water at Room Temperature. Angewandte Chemie - International Edition, 2016, 55, 4914-4918.	7.2	138
8	Discovery of technical methanation catalysts based on computational screening. Topics in Catalysis, 2007, 45, 9-13.	1.3	114
9	The effect of ionic strength on oil adhesion in sandstone â€“ the search for the low salinity mechanism. Scientific Reports, 2015, 5, 9933.	1.6	110
10	Functional Group Adsorption on Calcite: I. Oxygen Containing and Nonpolar Organic Molecules. Journal of Physical Chemistry C, 2016, 120, 16586-16596.	1.5	89
11	Structure of Nanoparticles Derived from Designer Surfactant TPGSâ€750â€M in Water, As Used in Organic Synthesis. Chemistry - A European Journal, 2018, 24, 6778-6786.	1.7	76
12	Energies of the Adsorption of Functional Groups to Calcium Carbonate Polymorphs: The Importance of â^'OH and â^'COOH Groups. Langmuir, 2013, 29, 11062-11073.	1.6	75
13	Elements of Eoarchean life trapped in mineral inclusions. Nature, 2017, 548, 78-81.	13.7	75
14	Hydrogen sulfide capture and removal technologies: A comprehensive review of recent developments and emerging trends. Separation and Purification Technology, 2022, 298, 121448.	3.9	70
15	Macroscopic Alignment of Silver Nanoparticles in Reverse Hexagonal Liquid Crystalline Templates. Nano Letters, 2002, 2, 1403-1407.	4.5	69
16	Probing the Surface Charge on the Basal Planes of Kaolinite Particles with High-Resolution Atomic Force Microscopy. Langmuir, 2017, 33, 14226-14237.	1.6	65
17	Micelle-enabled clean and selective sulfonylation of polyfluoroarenes in water under mild conditions. Green Chemistry, 2018, 20, 1784-1790.	4.6	65
18	How Naturally Adsorbed Material on Minerals Affects Low Salinity Enhanced Oil Recovery. Energy & Fuels, 2014, 28, 4849-4858.	2.5	60

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19	Surface Tension Alteration on Calcite, Induced by Ion Substitution. Journal of Physical Chemistry C, 2014, 118, 3078-3087.	1.5	58
20	The mechanisms of crystal growth inhibition by organic and inorganic inhibitors. Nature Communications, 2018, 9, 1578.	5.8	57
21	First-Principles Prediction of Liquid/Liquid Interfacial Tension. Journal of Chemical Theory and Computation, 2014, 10, 3401-3408.	2.3	56
22	Modelling how incorporation of divalent cations affects calcite wettabilityâ€“implications for biomineralisation and oil recovery. Scientific Reports, 2016, 6, 28854.	1.6	53
23	Virtual reality in chemical and biochemical engineering education and training. Education for Chemical Engineers, 2021, 36, 143-153.	2.8	52
24	Functional Group Adsorption on Calcite: II. Nitrogen and Sulfur Containing Organic Molecules. Journal of Physical Chemistry C, 2016, 120, 16597-16607.	1.5	48
25	Surfactant Technology: With New Rules, Designing New Sequences Is Required!. Organic Process Research and Development, 2020, 24, 841-849.	1.3	47
26	Titanium dioxide thin-film growth on silicon (111) by chemical vapor deposition of titanium(IV) isopropoxide. Journal of Applied Physics, 2002, 92, 3381-3387.	1.1	45
27	Self Blocking of CO Dissociation on a Stepped Ruthenium Surface. Topics in Catalysis, 2010, 53, 357-364.	1.3	44
28	Predicting the pK_a and Stability of Organic Acids and Bases at an Oilâ€“Water Interface. Langmuir, 2014, 30, 6437-6445.	1.6	43
29	Metalorganic chemical vapor deposition of anatase titanium dioxide on Si: Modifying the interface by pre-oxidation. Surface Science, 2003, 530, 63-70.	0.8	42
30	Hydrolytic Stability of 3-Aminopropylsilane Coupling Agent on Silica and Silicate Surfaces at Elevated Temperatures. ACS Applied Materials & Interfaces, 2017, 9, 8344-8353.	4.0	41
31	Electronic structure of lithium-doped anataseTiO2prepared in ultrahigh vacuum. Physical Review B, 2005, 71, .	1.1	39
32	Calculation of Entropy of Adsorption for Small Molecules on Mineral Surfaces. Journal of Physical Chemistry C, 2018, 122, 8236-8243.	1.5	38
33	Density Functional Theory with Modified Dispersion Correction for Metals Applied to Self-Assembled Monolayers of Thiols on Au(111). Journal of Theoretical Chemistry, 2013, 2013, 1-9.	1.5	37
34	Adsorption and Charge-Transfer Study of Bi-isonicotinic Acid on In Situ-Grown Anatase TiO2Nanoparticles. Journal of Physical Chemistry B, 2004, 108, 3114-3122.	1.2	35
35	How acidic is water on calcite?. Journal of Physical Chemistry C, 2012, 116, 18779-18787.	1.5	34
36	High surface area calcite. Journal of Crystal Growth, 2013, 371, 34-38.	0.7	33

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37	Strontium, Nickel, Cadmium, and Lead Substitution into Calcite, Studied by Density Functional Theory. Langmuir, 2014, 30, 6129-6133.	1.6	33
38	Hybrid machine learning assisted modelling framework for particle processes. Computers and Chemical Engineering, 2020, 140, 106916.	2.0	33
39	Calcite Growth Kinetics: Dependence on Saturation Index, Ca²⁺:CO₃^{2â€“} Activity Ratio, and Surface Atomic Structure. Crystal Growth and Design, 2016, 16, 3602-3612.	1.4	30
40	A Rhodium-Based Methane Oxidation Catalyst with High Tolerance to H₂O and SO₂. ACS Catalysis, 2020, 10, 1821-1827.	5.5	29
41	Li insertion in thin film anatase TiO2: identification of a two-phase regime with photoelectron spectroscopy. Chemical Physics Letters, 2002, 360, 85-90.	1.2	26
42	Incorporation of Monovalent Cations in Sulfate Green Rust. Inorganic Chemistry, 2014, 53, 8887-8894.	1.9	26
43	Quantum computing for chemical and biomolecular product design. Current Opinion in Chemical Engineering, 2022, 36, 100754.	3.8	26
44	Fundamental, Binary Combination, and Overtone Modes in Methoxy Adsorbed on Cu(100):Â Infrared Spectroscopy and Ab Initio Calculations. Journal of Physical Chemistry B, 2002, 106, 5200-5211.	1.2	25
45	Salinity-Dependent Adhesion Response Properties of Aluminosilicate (K-Feldspar) Surfaces. Energy & Fuels, 2017, 31, 4670-4680.	2.5	25
46	A Microkinetic Model of Calcite Step Growth. Angewandte Chemie - International Edition, 2016, 55, 11086-11090.	7.2	24
47	Transformation of Pyridine to Î±-Pyridyl on W(110) As Probed by Vibrational Spectroscopy:Â Experiments and Calculations. Journal of Physical Chemistry B, 2001, 105, 9458-9462.	1.2	23
48	Predicting hydration energies for multivalent ions. Journal of Computational Chemistry, 2014, 35, 2070-2075.	1.5	23
49	Is bicarbonate stable in and on the calcite surface?. Geochimica Et Cosmochimica Acta, 2016, 176, 198-205.	1.6	23
50	Infrared Spectroscopy and Density Functional Theory Investigation of Calcite, Chalk, and Coccolithsâ€”Do We Observe the Mineral Surface?. Journal of Physical Chemistry A, 2014, 118, 10720-10729.	1.1	22
51	Calcite Wettability in the Presence of Dissolved Mg²⁺ and SO₄^{2â€“}. Energy & Fuels, 2017, 31, 1005-1014.	2.5	22
52	Insights into the Pore-Scale Mechanism for the Low-Salinity Effect: Implications for Enhanced Oil Recovery. Energy & Fuels, 2018, 32, 12081-12090.	2.5	21
53	Adhesion of Alkane as a Functional Group on Muscovite and Quartz: Dependence on pH and Contact Time. Langmuir, 2014, 30, 14476-14485.	1.6	20
54	Density functional theory with modified dispersion correction for metals applied to molecular adsorption on Pt(111). Physical Chemistry Chemical Physics, 2016, 18, 19118-19122.	1.3	20

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55	HandaPhos: A General Ligand Enabling Sustainable ppm Levels of Palladium-Catalyzed Cross-Couplings in Water at Room Temperature. Angewandte Chemie, 2016, 128, 4998-5002.	1.6	20
56	Sulfur poisoning and regeneration of Rh-ZSM-5 catalysts for total oxidation of methane. Applied Catalysis B: Environmental, 2020, 277, 119176.	10.8	20
57	A Microkinetic Model of Calcite Step Growth. Angewandte Chemie, 2016, 128, 11252-11256.	1.6	18
58	A Quantum Mechanically Derived Force Field To Predict CO₂ Adsorption on Calcite {10.4} in an Aqueous Environment. Journal of Physical Chemistry C, 2017, 121, 24025-24035.	1.5	18
59	Tailor-made solvents for pharmaceutical use? Experimental and computational approach for determining solubility in deep eutectic solvents (DES). International Journal of Pharmaceutics: X, 2019, 1, 100034.	1.2	18
60	Could Atomic-Force Microscopy Force Mapping Be a Fast Alternative to Core-Plug Tests for Optimizing Injection-Water Salinity for Enhanced Oil Recovery in Sandstone?. SPE Journal, 2016, 21, 0720-0729.	1.7	17
61	Ion effects on molecular interaction between graphene oxide and organic molecules. Environmental Science: Nano, 2019, 6, 2281-2291.	2.2	17
62	Integration of first-principle models and machine learning in a modeling framework: An application to flocculation. Chemical Engineering Science, 2021, 245, 116864.	1.9	17
63	TiO2 chemical vapor deposition on Si(111) in ultrahigh vacuum: Transition from interfacial phase to crystalline phase in the reaction limited regime. Surface Science, 2011, 605, 1147-1156.	0.8	16
64	Phase separation and charge localization in UHV-lithiated anataseTiO2nanoparticles. Physical Review B, 2005, 71, .	1.1	15
65	First-Principles Prediction of Surface Wetting. Langmuir, 2020, 36, 12451-12459.	1.6	15
66	First-principles prediction of critical micellar concentrations for ionic and nonionic surfactants. Journal of Colloid and Interface Science, 2022, 606, 618-627.	5.0	14
67	Predicting pK_afor proteins using COSMO-RS. PeerJ, 2013, 1, e198.	0.9	14
68	UHV-MOCVD growth of TiO2 on SiOx/Si(111): Interfacial properties reflected in the Si 2p photoemission spectra. Surface Science, 2005, 580, 207-217.	0.8	13
69	Sensitivity Analysis of Cluster Models for Calculating Adsorption Energies for Organic Molecules on Mineral Surfaces. Journal of Physical Chemistry C, 2011, 115, 10044-10055.	1.5	13
70	Electronic-Structure-Based Design of Ordered Alloys. MRS Bulletin, 2006, 31, 986-990.	1.7	12
71	Carbide induced reconstruction of monatomic steps on Ni(111) â€“ A density functional study. Surface Science, 2007, 601, 649-655.	0.8	12
72	The effect of solvation and temperature on the adsorption of small organic molecules on calcite. Physical Chemistry Chemical Physics, 2018, 20, 7140-7147.	1.3	12

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73	Multiconfiguration Diracâ€“Hartreeâ€“Fock calculations for intercombination lines in silicon-like ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 503-508.	0.6	11
74	Surface-induced Câ€“O bond anharmonicity of methoxy adsorbed on Cu(100): Experiments and density-functional theory calculations. Journal of Chemical Physics, 2005, 123, 224714.	1.2	11
75	Predicting CO₂â€“H₂O Interfacial Tension Using COSMO-RS. Journal of Chemical Theory and Computation, 2017, 13, 804-810.	2.3	11
76	Prediction of aliphatic and aromatic oil-water interfacial tension at temperatures >100ÂÂ°C using COSMO-RS. Fluid Phase Equilibria, 2018, 476, 25-29.	1.4	11
77	Electrochemical and molecular modelling studies of CO2 corrosion inhibition characteristics of alkanolamine molecules for the protection of 1Cr steel. Corrosion Science, 2022, 195, 109999.	3.0	11
78	Surface chemistry of TiCl4 on clean and hydrogen modified W(): identification of surface intermediates. Surface Science, 2002, 521, 129-138.	0.8	9
79	First-Principle Calculations of the Experimental Vibrational Spectrum of a Surface Adsorbate: Anharmonic Resonance Coupling between Fundamental and Binary Modes. Physical Review Letters, 2003, 90, 076103.	2.9	9
80	Influence of the support on rhodium speciation and catalytic activity of rhodium-based catalysts for total oxidation of methane. Catalysis Science and Technology, 2020, 10, 6035-6044.	2.1	8
81	Specific ion effects on the hydrophobic interaction of benzene self-assembled monolayers. Physical Chemistry Chemical Physics, 2015, 17, 21432-21441.	1.3	7
82	Analysis of the competition between forbidden and hyperfine-induced transitions in Ne-like ions. Physical Review A, 2016, 93, .	1.0	7
83	Thermodynamic and Kinetic Parameters for Calcite Nucleation on Peptoid and Model Scaffolds: A Step toward Nacre Mimicry. Crystal Growth and Design, 2020, 20, 3762-3771.	1.4	7
84	Adsorption of nitrogen heterocyclic compounds (NHC) on soil minerals: Quinoline as an example. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 611, 125899.	2.3	7
85	Integration of Computational Chemistry and Artificial Intelligence for Multi-scale Modeling of Bioprocesses. Computer Aided Chemical Engineering, 2020, 48, 295-300.	0.3	6
86	Predicted structures of calcium aluminosilicate glass as a model for stone wool fiber: effects of composition and interatomic potential. Journal of Non-Crystalline Solids, 2021, 567, 120924.	1.5	6
87	Density Functional Theory Study on the Initial Reactions of D-Xylose and D-Xylulose Dehydration to Furfural. Carbohydrate Research, 2021, 511, 108463.	1.1	6
88	Lifetime calculations for the5s5pP23metastable level ofSr88I. Physical Review A, 2007, 75, .	1.0	5
89	InducingH/DExchange in Ultrathin Ice Films by Proton Deficiency. Physical Review Letters, 2011, 107, 216101.	2.9	5
90	The adsorption site of methoxy and ethoxy on Cu(100) as determined by vibrational spectroscopy and first principle calculations. Surface Science, 2004, 549, 87-96.	0.8	4

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91	Modular and intensified â€" Reimagining manufacturing at the energy-chemistry nexus and beyond. Chemical Engineering and Processing: Process Intensification, 2022, 174, 108883.	1.8	4
92	Anharmonic resonances in the Câ€"H stretch region of ethoxy adsorbed on W(): vibrational spectroscopy and calculations. Surface Science, 2003, 532-535, 221-226.	0.8	3
93	Interfacial tension in water/n-decane/naphthenic acid systems predicted by a combined COSMO-RS theory and pendant drop experimental study. Molecular Physics, 2020, 118, e1764645.	0.8	3
94	Implementation of first-principles surface interactions in a hybrid machine learning assisted modelling of flocculation. Computer Aided Chemical Engineering, 2021, , 845-850.	0.3	3
95	Unstable, Super Critical CO2â€"Water Displacement in Fine Grained Porous Media under Geologic Carbon Sequestration Conditions. Scientific Reports, 2019, 9, 11272.	1.6	2
96	Modeling of Liquid-Liquid Phase Transfer Catalysis: Process Intensification via Integration of Process Systems Engineering and Computational Chemistry. Computer Aided Chemical Engineering, 2020, , 43-48.	0.3	2
97	Molecular tracking: A concept for sideâ€draw distillation column design. AICHE Journal, 2021, 67, .	1.8	2
98	Towards a Rational, Quantum-Chemistry-Based Selection and Screening of Green Solvents for Liquid-Liquid Phase Transfer Catalysis. Computer Aided Chemical Engineering, 2021, 50, 1593-1598.	0.3	2
99	A density functional theory study of Fe(II)/Fe(III) distribution in single layer green rust: a cluster approach. Geochemical Transactions, 2021, 22, 3.	1.8	2
100	Molecular Transport across Oilâ€"Brine Interfaces Impacts Interfacial Tension: Time-Effects in Buoyant and Pendant Drop Measurements. Langmuir, 2021, 37, 585-595.	1.6	2
101	The Vibrational Spectra of Methyl Groups in Methylthiolate and Methoxy Adsorbed on Cu(100). Langmuir, 2002, 18, 3759-3762.	1.6	1
102	Predicting Interfacial Tension Of Multiphase Systems Based On Computational Single-Molecule Quantum Mechanics And Thermodynamics Applying Four Different Physical Models And COSMO-Theory. , 2014, , .		1
103	Titelbild: HandaPhos: A General Ligand Enabling Sustainable ppm Levels of Palladium-Catalyzed Cross-Couplings in Water at Room Temperature (Angew. Chem. 16/2016). Angewandte Chemie, 2016, 128, 4921-4921.	1.6	1