# Martin Andersson

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | 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 |
| 2 | Quantum computing for chemical and biomolecular product design. Current Opinion in Chemical Engineering, 2022, 36, 100754. | 3.8 | 26 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | Molecular tracking: A concept for sideâ€draw distillation column design. AICHE Journal, 2021, 67, . | 1.8 | 2 |
| 7 | 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 |
| 8 | 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 |
| 9 | 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 |
| 10 | 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 |
| 11 | Virtual reality in chemical and biochemical engineering education and training. Education for Chemical Engineers, 2021, 36, 143-153. | 2.8 | 52 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | A Rhodium-Based Methane Oxidation Catalyst with High Tolerance to H<sub>2</sub>O and SO<sub>2</sub>. ACS Catalysis, 2020, 10, 1821-1827. | 5.5 | 29 |
| 17 | Surfactant Technology: With New Rules, Designing New Sequences Is Required!. Organic Process Research and Development, 2020, 24, 841-849. | 1.3 | 47 |
| 18 | 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 |

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|---|---|---|---|
| 19 | Integration of Computational Chemistry and Artificial Intelligence for Multi-scale Modeling of Bioprocesses. Computer Aided Chemical Engineering, 2020, 48, 295-300. | 0.3 | 6 |
| 20 | First-Principles Prediction of Surface Wetting. Langmuir, 2020, 36, 12451-12459. | 1.6 | 15 |
| 21 | 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 |
| 22 | Sulfur poisoning and regeneration of Rh-ZSM-5 catalysts for total oxidation of methane. Applied Catalysis B: Environmental, 2020, 277, 119176. | 10.8 | 20 |
| 23 | 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 |
| 24 | 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 |
| 25 | Hybrid machine learning assisted modelling framework for particle processes. Computers and Chemical Engineering, 2020, 140, 106916. | 2.0 | 33 |
| 26 | Unstable, Super Critical CO2â€“Water Displacement in Fine Grained Porous Media under Geologic Carbon Sequestration Conditions. Scientific Reports, 2019, 9, 11272. | 1.6 | 2 |
| 27 | 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 |
| 28 | Ion effects on molecular interaction between graphene oxide and organic molecules. Environmental Science: Nano, 2019, 6, 2281-2291. | 2.2 | 17 |
| 29 | 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 |
| 30 | 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 |
| 31 | The mechanisms of crystal growth inhibition by organic and inorganic inhibitors. Nature Communications, 2018, 9, 1578. | 5.8 | 57 |
| 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 | Micelle-enabled clean and selective sulfonylation of polyfluoroarenes in water under mild conditions. Green Chemistry, 2018, 20, 1784-1790. | 4.6 | 65 |
| 34 | 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 |
| 35 | 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 |
| 36 | Predicting CO<sub>2</sub>â€“H<sub>2</sub>O Interfacial Tension Using COSMO-RS. Journal of Chemical Theory and Computation, 2017, 13, 804-810. | 2.3 | 11 |

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| 37 | 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 |
| 38 | Salinity-Dependent Adhesion Response Properties of Aluminosilicate (K-Feldspar) Surfaces. Energy & Fuels, 2017, 31, 4670-4680. | 2.5 | 25 |
| 39 | Calcite Wettability in the Presence of Dissolved Mg<sup>2+</sup> and SO<sub>4</sub><sup>2â€“</sup>. Energy & Fuels, 2017, 31, 1005-1014. | 2.5 | 22 |
| 40 | A Quantum Mechanically Derived Force Field To Predict CO<sub>2</sub> Adsorption on Calcite {10.4} in an Aqueous Environment. Journal of Physical Chemistry C, 2017, 121, 24025-24035. | 1.5 | 18 |
| 41 | Elements of Eoarchean life trapped in mineral inclusions. Nature, 2017, 548, 78-81. | 13.7 | 75 |
| 42 | 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 |
| 43 | Functional Group Adsorption on Calcite: I. Oxygen Containing and Nonpolar Organic Molecules. Journal of Physical Chemistry C, 2016, 120, 16586-16596. | 1.5 | 89 |
| 44 | Functional Group Adsorption on Calcite: II. Nitrogen and Sulfur Containing Organic Molecules. Journal of Physical Chemistry C, 2016, 120, 16597-16607. | 1.5 | 48 |
| 45 | 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 |
| 46 | 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 |
| 47 | Calcite Growth Kinetics: Dependence on Saturation Index, Ca<sup>2+</sup>:CO<sub>3</sub><sup>2â€“</sup> Activity Ratio, and Surface Atomic Structure. Crystal Growth and Design, 2016, 16, 3602-3612. | 1.4 | 30 |
| 48 | A Microkinetic Model of Calcite Step Growth. Angewandte Chemie - International Edition, 2016, 55, 11086-11090. | 7.2 | 24 |
| 49 | A Microkinetic Model of Calcite Step Growth. Angewandte Chemie, 2016, 128, 11252-11256. | 1.6 | 18 |
| 50 | Modelling how incorporation of divalent cations affects calcite wettabilityâ€“implications for biomineralisation and oil recovery. Scientific Reports, 2016, 6, 28854. | 1.6 | 53 |
| 51 | Analysis of the competition between forbidden and hyperfine-induced transitions in Ne-like ions. Physical Review A, 2016, 93, . | 1.0 | 7 |
| 52 | 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 |
| 53 | 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 |
| 54 | 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 |

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| 55 | Is bicarbonate stable in and on the calcite surface?. Geochimica Et Cosmochimica Acta, 2016, 176, 198-205. | 1.6 | 23 |
| 56 | 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 |
| 57 | Specific ion effects on the hydrophobic interaction of benzene self-assembled monolayers. Physical Chemistry Chemical Physics, 2015, 17, 21432-21441. | 1.3 | 7 |
| 58 | 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 |
| 59 | Predicting hydration energies for multivalent ions. Journal of Computational Chemistry, 2014, 35, 2070-2075. | 1.5 | 23 |
| 60 | 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 |
| 61 | Predicting the pK<sub>a</sub> and Stability of Organic Acids and Bases at an Oilâ€“Water Interface. Langmuir, 2014, 30, 6437-6445. | 1.6 | 43 |
| 62 | 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 |
| 63 | How Naturally Adsorbed Material on Minerals Affects Low Salinity Enhanced Oil Recovery. Energy & Fuels, 2014, 28, 4849-4858. | 2.5 | 60 |
| 64 | Incorporation of Monovalent Cations in Sulfate Green Rust. Inorganic Chemistry, 2014, 53, 8887-8894. | 1.9 | 26 |
| 65 | First-Principles Prediction of Liquid/Liquid Interfacial Tension. Journal of Chemical Theory and Computation, 2014, 10, 3401-3408. | 2.3 | 56 |
| 66 | Strontium, Nickel, Cadmium, and Lead Substitution into Calcite, Studied by Density Functional Theory. Langmuir, 2014, 30, 6129-6133. | 1.6 | 33 |
| 67 | Surface Tension Alteration on Calcite, Induced by Ion Substitution. Journal of Physical Chemistry C, 2014, 118, 3078-3087. | 1.5 | 58 |
| 68 | Direct observation of ionic structure at solid-liquid interfaces: a deep look into the Stern Layer. Scientific Reports, 2014, 4, 4956. | 1.6 | 160 |
| 69 | 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 |
| 70 | High surface area calcite. Journal of Crystal Growth, 2013, 371, 34-38. | 0.7 | 33 |
| 71 | 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 |
| 72 | Predicting pK<sub>a</sub>for proteins using COSMO-RS. PeerJ, 2013, 1, e198. | 0.9 | 14 |

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| 73 | How acidic is water on calcite?. Journal of Physical Chemistry C, 2012, 116, 18779-18787. | 1.5 | 34 |
| 74 | 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 |
| 75 | 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 |
| 76 | InducingH/DExchange in Ultrathin Ice Films by Proton Deficiency. Physical Review Letters, 2011, 107, 216101. | 2.9 | 5 |
| 77 | Self Blocking of CO Dissociation on a Stepped Ruthenium Surface. Topics in Catalysis, 2010, 53, 357-364. | 1.3 | 44 |
| 78 | Structure sensitivity of the methanation reaction: H2-induced CO dissociation on nickel surfaces. Journal of Catalysis, 2008, 255, 6-19. | 3.1 | 411 |
| 79 | First principles calculations and experimental insight into methane steam reforming over transition metal catalysts. Journal of Catalysis, 2008, 259, 147-160. | 3.1 | 559 |
| 80 | Lifetime calculations for the5s5pP23metastable level ofSr88I. Physical Review A, 2007, 75, . | 1.0 | 5 |
| 81 | Carbide induced reconstruction of monatomic steps on Ni(111) â€“ A density functional study. Surface Science, 2007, 601, 649-655. | 0.8 | 12 |
| 82 | 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 |
| 83 | Discovery of technical methanation catalysts based on computational screening. Topics in Catalysis, 2007, 45, 9-13. | 1.3 | 114 |
| 84 | Toward computational screening in heterogeneous catalysis: Pareto-optimal methanation catalysts. Journal of Catalysis, 2006, 239, 501-506. | 3.1 | 314 |
| 85 | Electronic-Structure-Based Design of Ordered Alloys. MRS Bulletin, 2006, 31, 986-990. | 1.7 | 12 |
| 86 | 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 |
| 87 | 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 |
| 88 | Phase separation and charge localization in UHV-lithiated anataseTiO2nanoparticles. Physical Review B, 2005, 71, . | 1.1 | 15 |
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| 90 | 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 |

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| 91 | Electronic structure of lithium-doped anataseTiO2prepared in ultrahigh vacuum. Physical Review B, 2005, 71, . | 1.1 | 39 |
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| 93 | 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 |
| 94 | 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 |
| 95 | 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 |
| 96 | 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 |
| 97 | 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 |
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| 99 | The Vibrational Spectra of Methyl Groups in Methylthiolate and Methoxy Adsorbed on Cu(100). Langmuir, 2002, 18, 3759-3762. | 1.6 | 1 |
| 100 | Macroscopic Alignment of Silver Nanoparticles in Reverse Hexagonal Liquid Crystalline Templates. Nano Letters, 2002, 2, 1403-1407. | 4.5 | 69 |
| 101 | Surface chemistry of TiCl4 on clean and hydrogen modified W(): identification of surface intermediates. Surface Science, 2002, 521, 129-138. | 0.8 | 9 |
| 102 | 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 |
| 103 | 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 |