James D Kubicki

List of Publications by Year
in descending order

188 papers	9,968 citations	23567 58 h-index	43889 91 g-index
206 all docs	206 docs citations	206 times ranked	10362 citing authors

#	Article	IF	Citations
1	Molecular orbital study of Fe(II) and Fe(III) complexation with salicylate and citrate ligands: Implications for soil biogeochemistry. Soil Science Society of America Journal, 2022, 86, 181-194.	2.2	3
2	Connecting Thermodynamics of Alkali Ion Exchange on the Quartz (101) Surface with Density Functional Theory Calculations. Journal of Physical Chemistry A, 2022, 126, 4286-4294.	2.5	2
3	Equilibrium and kinetic isotopic fractionation in the CO2 hydration and hydroxylation reactions: Analysis of the role of hydrogen-bonding via quantum mechanical calculations. Geochimica Et Cosmochimica Acta, 2021, 292, 37-63.	3.9	9
4	Density Functional Tight-Binding Simulations Reveal the Presence of Surface Defects on the Quartz (101)â€"Water Interface. Journal of Physical Chemistry C, 2021, 125, 16246-16255.	3.1	4
5	Density Functional Theory Predictions of Noncovalent Hydrogen Isotope Effects during Octane Sorption to a Kaolinite Surface. ACS Earth and Space Chemistry, 2020, 4, 1756-1764.	2.7	1
6	In silico structure prediction of full-length cotton cellulose synthase protein (GhCESA1) and its hierarchical complexes. Cellulose, 2020, 27, 5597-5616.	4.9	13
7	A density functional theory study on the shape of the primary cellulose microfibril in plants: effects of C6 exocyclic group conformation and H-bonding. Cellulose, 2020, 27, 2389-2402.	4.9	29
8	In Situ and Real-Time ATR-FTIR Temperature-Dependent Adsorption Kinetics Coupled with DFT Calculations of Dimethylarsinate and Arsenate on Hematite Nanoparticles. Langmuir, 2020, 36, 4299-4307.	3.5	19
9	Integrating Density Functional Theory Modeling with Experimental Data to Understand and Predict Sorption Reactions: Exchange of Salicylate for Phosphate on Goethite. Soil Systems, 2020, 4, 27.	2.6	9
10	Adsorption of Organic Acids and Phosphate to an Iron (Oxyhydr)oxide Mineral: A Combined Experimental and Density Functional Theory Study. Journal of Physical Chemistry A, 2020, 124, 3249-3260.	2.5	9
11	Gibbsite (100) and Kaolinite (100) Sorption of Cadmium(II): A Density Functional Theory and XANES Study of Structures and Energies. Journal of Physical Chemistry A, 2019, 123, 6319-6333.	2.5	9
12	Evaluating Computational Chemistry Methods for Isotopic Fractionation between CO2(g) and H2O(g). Journal of Chemical Information and Modeling, 2019, 59, 4663-4677.	5.4	1
13	Integrating Density Functional Theory Calculations with Vibrational and Nuclear Magnetic Resonance Spectroscopy. ACS Symposium Series, 2019, , 89-102.	0.5	0
14	Probing cellulose structures with vibrational spectroscopy. Cellulose, 2019, 26, 35-79.	4.9	132
15	Quantum Mechanical Modeling of the Vibrational Spectra of Minerals with a Focus on Clays. Minerals (Basel, Switzerland), 2019, 9, 141.	2.0	18
16	Simulations of Cellulose Synthesis Initiation and Termination in Bacteria. Journal of Physical Chemistry B, 2019, 123, 3699-3705.	2.6	10
17	Adsorption Study of Al³⁺, Cr³⁺, and Mn²⁺ onto Quartz and Corundum using Flow Microcalorimetry, Quartz Crystal Microbalance, and Density Functional Theory. ACS Earth and Space Chemistry, 2019, 3, 432-441.	2.7	16
18	Simultaneous Adsorption and Incorporation of Sr²⁺ at the Barite (001)â€"Water Interface. Journal of Physical Chemistry C, 2019, 123, 1194-1207.	3.1	21

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19	Arabinose substitution effect on xylan rigidity and self-aggregation. Cellulose, 2019, 26, 2267-2278.	4.9	31
20	Quantum Calculations on Plant Cell Wall Component Interactions. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 485-495.	3.6	10
21	Initiation, Elongation, and Termination of Bacterial Cellulose Synthesis. ACS Omega, 2018, 3, 2690-2698.	3.5	23
22	An evaluation of the structures of cellulose generated by the CHARMM force field: comparisons to in planta cellulose. Cellulose, 2018, 25, 3755-3777.	4.9	20
23	Structure and reactivity of oxalate surface complexes on lepidocrocite derived from infrared spectroscopy, DFT-calculations, adsorption, dissolution and photochemical experiments. Geochimica Et Cosmochimica Acta, 2018, 226, 244-262.	3.9	37
24	Binding Geometries of Silicate Species on Ferrihydrite Surfaces. ACS Earth and Space Chemistry, 2018, 2, 125-134.	2.7	27
25	Density functional theory modeling of chromate adsorption onto ferrihydrite nanoparticles. Geochemical Transactions, 2018, 19, 8.	0.7	26
26	Structural factors affecting 13C NMR chemical shifts of cellulose: a computational study. Cellulose, 2018, 25, 23-36.	4.9	45
27	Reaction Mechanisms and Solidâ€"Gas Phase Reactions: Theory and Density Functional Theory Simulations. Reviews in Mineralogy and Geochemistry, 2018, 84, 85-101.	4.8	6
28	3. Reaction Mechanisms and Solidâ€"Gas Phase Reactions: Theory and Density Functional Theory Simulations. , 2018, , 85-102.		0
29	The Shape of Native Plant Cellulose Microfibrils. Scientific Reports, 2018, 8, 13983.	3.3	86
30	Kinetic analysis of cellulose synthase of Gluconacetobacter hansenii in whole cells and in purified form. Enzyme and Microbial Technology, 2018, 119, 24-29.	3.2	1
31	An integrated flow microcalorimetry, infrared spectroscopy and density functional theory approach to the study of chromate complexation on hematite and ferrihdyrite. Chemical Geology, 2017, 464, 23-33.	3.3	26
32	Fourier-transform infrared spectroscopy (FTIR) analysis of triclinic and hexagonal birnessites. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 178, 32-46.	3.9	40
33	Interactions between aromatic hydrocarbons and functionalized C₆₀ fullerenes â€" insights from experimental data and molecular modelling. Environmental Science: Nano, 2017, 4, 1045-1053.	4.3	17
34	Effect of amino acids on the precipitation kinetics and Ca isotopic composition of gypsum. Geochimica Et Cosmochimica Acta, 2017, 218, 343-364.	3.9	20
35	A density functional theory investigation of oxalate and Fe(II) adsorption onto the (010) goethite surface with implications for ligand- and reduction-promoted dissolution. Chemical Geology, 2017, 464, 14-22.	3.3	41
36	X-ray Absorption Spectroscopic Quantification and Speciation Modeling of Sulfate Adsorption on Ferrihydrite Surfaces. Environmental Science & Technology, 2016, 50, 8067-8076.	10.0	96

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37	Cellulose Structural Polymorphism in Plant Primary Cell Walls Investigated by High-Field 2D Solid-State NMR Spectroscopy and Density Functional Theory Calculations. Biomacromolecules, 2016, 17, 2210-2222.	5.4	94
38	Spectroscopy and Ultrafast Vibrational Dynamics of Strongly Hydrogen Bonded OH Species at the Î±-Al₂O₃(112Ì…0)/H₂O Interface. Journal of Physical Chemistry C, 2016, 120, 16153-16161.	3.1	42
39	Competitive Adsorption of Acetic Acid and Water on Kaolinite. Journal of Physical Chemistry A, 2016, 120, 8339-8346.	2.5	14
40	Effect of Ions on H-Bond Structure and Dynamics at the Quartz(101)â€“Water Interface. Langmuir, 2016, 32, 11353-11365.	3.5	41
41	Sustainable development of a surface-functionalized mesoporous aluminosilicate with ultra-high ion exchange efficiency. Inorganic Chemistry Frontiers, 2016, 3, 502-513.	6.0	23
42	DENSITY FUNCTIONAL THEORY MODELING OF FERRIHYDRITE NANOPARTICLE OXYANION ADSORPTION. , 2016, , .		1
43	Hydrogen-Bonding Network and OH Stretch Vibration of Cellulose: Comparison of Computational Modeling with Polarized IR and SFG Spectra. Journal of Physical Chemistry B, 2015, 119, 15138-15149.	2.6	152
44	Experimental Study of Strontium Adsorption on Anatase Nanoparticles as a Function of Size with a Density Functional Theory and CD Model Interpretation. Langmuir, 2015, 31, 703-713.	3.5	12
45	Rb⁺ Adsorption at the Quartz(101)â€“Aqueous Interface: Comparison of Resonant Anomalous X-ray Reflectivity with ab Initio Calculations. Journal of Physical Chemistry C, 2015, 119, 4778-4788.	3.1	34
46	Plagioclase Dissolution during CO₂â€“SO₂ Cosequestration: Effects of Sulfate. Environmental Science & Technology, 2015, 49, 1946-1954.	10.0	23
47	How Cellulose Elongatesâ€”A QM/MM Study of the Molecular Mechanism of Cellulose Polymerization in Bacterial CESA. Journal of Physical Chemistry B, 2015, 119, 6525-6535.	2.6	13
48	Constraints on $${m I}eta$$ I Î² cellulose twist from DFT calculations of $$^{13}hbox {C}$$ 13 C NMR chemical shifts. Cellulose, 2014, 21, 3979-3991.	4.9	14
49	Quantum mechanical modeling of hydrolysis and H2O-exchange in Mg-, Ca-, and Ni-silicate clusters: Implications for dissolution mechanisms of olivine minerals. American Mineralogist, 2014, 99, 2303-2312.	1.9	12
50	Arsenic Adsorption onto Minerals: Connecting Experimental Observations with Density Functional Theory Calculations. Minerals (Basel, Switzerland), 2014, 4, 208-240.	2.0	58
51	Quantum mechanical calculations on celluloseâ€“water interactions: structures, energetics, vibrational frequencies and NMR chemical shifts for surfaces of IÎ± and IÎ² cellulose. Cellulose, 2014, 21, 909-926.	4.9	27
52	A DFT study of vibrational frequencies and 13C NMR chemical shifts of model cellulosic fragments as a function of size. Cellulose, 2014, 21, 53-70.	4.9	21
53	Vibrational Density of States of Strongly H-Bonded Interfacial Water: Insights from Inelastic Neutron Scattering and Theory. Journal of Physical Chemistry C, 2014, 118, 10805-10813.	3.1	48
54	Stereochemistry, elution order and molecular modeling of four diaergostanes in petroleum. Organic Geochemistry, 2014, 76, 1-8.	1.8	12

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55	Towards lignin-protein crosslinking: amino acid adducts of a lignin model quinone methide. Cellulose, 2014, 21, 1395-1407.	4.9	8
56	Molecular dynamics simulation study of xyloglucan adsorption on cellulose surfaces: effects of surface hydrophobicity and side-chain variation. Cellulose, 2014, 21, 1025-1039.	4.9	86
57	Molecular level investigations of phosphate sorption on corundum (Î±-Al2O3) by 31P solid state NMR, ATR-FTIR and quantum chemical calculation. Geochimica Et Cosmochimica Acta, 2013, 107, 252-266.	3.9	94
58	Adsorption of carbon dioxide on Al/Fe oxyhydroxide. Journal of Colloid and Interface Science, 2013, 400, 1-10.	9.4	22
59	Cellulose Microfibril Twist, Mechanics, and Implication for Cellulose Biosynthesis. Journal of Physical Chemistry A, 2013, 117, 2580-2589.	2.5	79
60	Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems. Langmuir, 2013, 29, 7838-7846.	3.5	96
61	In Situ Structural Characterization of Ferric Iron Dimers in Aqueous Solutions: Identification of Î¼-Oxo Species. Inorganic Chemistry, 2013, 52, 6788-6797.	4.0	51
62	Sum-Frequency-Generation Vibration Spectroscopy and Density Functional Theory Calculations with Dispersion Corrections (DFT-D2) for Cellulose Iâ± and Iâ². Journal of Physical Chemistry B, 2013, 117, 6681-6692.	2.6	90
63	Anatase Nanoparticle Surface Reactivity in NaCl Media: A CDâ€“MUSIC Model Interpretation of Combined Experimental and Density Functional Theory Studies. Langmuir, 2013, 29, 8572-8583.	3.5	11
64	Identification and Characterization of a Cellulose Binding Heptapeptide Revealed by Phage Display. Biomacromolecules, 2013, 14, 1795-1805.	5.4	35
65	Single-Site and Monolayer Surface Hydration Energy of Anatase and Rutile Nanoparticles Using Density Functional Theory. Journal of Physical Chemistry C, 2013, 117, 26084-26090.	3.1	18
66	Quantum mechanical modeling of the structures, energetics and spectral properties of Iâ± and Iâ² cellulose. Cellulose, 2013, 20, 9-23.	4.9	39
67	Modeling Water Adsorption on Rutile (110) Using van der Waals Density Functional and DFT+U Methods. Journal of Physical Chemistry C, 2013, 117, 23638-23644.	3.1	33
68	Tertiary model of a plant cellulose synthase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 7512-7517.	7.1	163
69	Molecular dynamics simulations of the interactions between TiO₂ nanoparticles and water with Na⁺ and Cl^{âˆ’}, methanol, and formic acid using a reactive force field. Journal of Materials Research, 2013, 28, 513-520.	2.6	58
70	ATRâ€“FTIR and Density Functional Theory Study of the Structures, Energetics, and Vibrational Spectra of Phosphate Adsorbed onto Goethite. Langmuir, 2012, 28, 14573-14587.	3.5	142
71	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	3.2	46
72	Quantum mechanical calculations on FeOH nanoparticles. Geoderma, 2012, 189-190, 236-242.	5.1	10

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73	A New Hypothesis for the Dissolution Mechanism of Silicates. Journal of Physical Chemistry C, 2012, 116, 17479-17491.	3.1	52
74	Molecular models of birnessite and related hydrated layered minerals. American Mineralogist, 2012, 97, 1505-1514.	1.9	36
75	In search of OHâ€"Ï€ interactions between 1-methylimidazole and water using a combined computational quantum chemistry and ATR-FTIR spectroscopy approach. Journal of Molecular Structure, 2012, 1026, 78-87.	3.6	6
76	Adsorption of Nitrate on Kaolinite Surfaces: A Theoretical Study. Journal of Physical Chemistry B, 2012, 116, 11266-11273.	2.6	20
77	Evaluation of potential reaction mechanisms leading to the formation of coniferyl alcohol Î±-linkages in lignin: a density functional theory study. Physical Chemistry Chemical Physics, 2011, 13, 20974.	2.8	14
78	Evaluating Glutamate and Aspartate Binding Mechanisms to Rutile (Î±-TiO₂) via ATR-FTIR Spectroscopy and Quantum Chemical Calculations. Langmuir, 2011, 27, 1778-1787.	3.5	65
79	Adsorption of Zn²⁺ on the (110) Surface of TiO₂ (Rutile): A Density Functional Molecular Dynamics Study. Journal of Physical Chemistry C, 2011, 115, 9608-9614.	3.1	12
80	Differential Pair Distribution Function Study of the Structure of Arsenate Adsorbed on Nanocrystalline Î³-Alumina. Environmental Science & Technology, 2011, 45, 9687-9692.	10.0	66
81	Comparison of Cation Adsorption by Isostructural Rutile and Cassiterite. Langmuir, 2011, 27, 4585-4593.	3.5	29
82	Comparison of Multistandard and TMS-Standard Calculated NMR Shifts for Coniferyl Alcohol and Application of the Multistandard Method to Lignin Dimers. Journal of Physical Chemistry B, 2011, 115, 1958-1970.	2.6	39
83	Aluminum coprecipitates with Fe (hydr)oxides: Does isomorphous substitution of Al3+ for Fe3+ in goethite occur?. Geochimica Et Cosmochimica Acta, 2011, 75, 4667-4683.	3.9	54
84	Simulations of the Quartz(101Ì…1)/Water Interface: A Comparison of Classical Force Fields, Ab Initio Molecular Dynamics, and X-ray Reflectivity Experiments. Journal of Physical Chemistry C, 2011, 115, 2076-2088.	3.1	183
85	Periodic Density Functional Theory Study of Water Adsorption on the Î±-Quartz (101) Surface. Journal of Physical Chemistry C, 2011, 115, 5756-5766.	3.1	73
86	Faster proton transfer dynamics of water on SnO2 compared to TiO2. Journal of Chemical Physics, 2011, 134, 044706.	3.0	34
87	Electronic structure, chemical bonding, and oxidation numbers of firstâ€row transition metals in [MePIm₂] complexes and their cations. International Journal of Quantum Chemistry, 2011, 111, 3630-3642.	2.0	1
88	Photoinduced activation of CO2 on TiO2 surfaces: Quantum chemical modeling of CO2 adsorption on oxygen vacancies. Fuel Processing Technology, 2011, 92, 805-811.	7.2	47
89	Interaction energy and the shift in OH stretch frequency on hydrogen bonding for the H₂O â†' H₂O, CH₃OH â†' H₂O, and H₂O â†' CH₃OH dimers. Journal of Computational Chemistry, 2010, 31, 963-972.	3.3	17
90	Reductive dissolution of ferrihydrite by ascorbic acid and the inhibiting effect of phospholipid. Journal of Colloid and Interface Science, 2010, 341, 215-223.	9.4	23

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91	Surface science studies of environmentally relevant iron (oxy)hydroxides ranging from the nano to the macro-regime. Surface Science, 2010, 604, 1065-1071.	1.9	6
92	MP2, density functional theory, and molecular mechanical calculations of Câ€“HÂ·Â·Â·Ï€ and hydrogen bond interactions in a cellulose-binding moduleâ€“cellulose model system. Carbohydrate Research, 2010, 345, 1741-1751.	2.3	30
93	Description of Mg²⁺ Release from Forsterite Using Ab Initio Methods. Journal of Physical Chemistry C, 2010, 114, 5417-5428.	3.1	20
94	Complexation of carboxyl groups in bacterial lipopolysaccharides: Interactions of H+, Mg2+, Ca2+, Cd2+, and UO22+ with Kdo and galacturonate molecules via quantum mechanical calculations and NMR spectroscopy. Chemical Geology, 2010, 273, 55-75.	3.3	9
95	Development of a Reactive Force Field for Ironâˆ’Oxyhydroxide Systems. Journal of Physical Chemistry A, 2010, 114, 6298-6307.	2.5	199
96	Surface Speciation of Phosphate on Boehmite (Î³-AlOOH) Determined from NMR Spectroscopy. Langmuir, 2010, 26, 4753-4761.	3.5	63
97	Photodissolution of Ferrihydrite in the Presence of Oxalic Acid: An In Situ ATR-FTIR/DFT Study. Langmuir, 2010, 26, 16246-16253.	3.5	53
98	Quantum mechanical calculation of aqueuous uranium complexes: carbonate, phosphate, organic and biomolecular species. Chemistry Central Journal, 2009, 3, 10.	2.6	64
99	Ferrihydrite reactivity toward carbon dioxide. Journal of Colloid and Interface Science, 2009, 337, 492-500.	9.4	79
100	Photoinduced activation of CO2 on Ti-based heterogeneous catalysts: Current state, chemical physics-based insights and outlook. Energy and Environmental Science, 2009, 2, 745.	30.8	653
101	Quantum Mechanical Modeling of CO₂Interactions with Irradiated Stoichiometric and Oxygen-Deficient Anatase TiO₂Surfaces: Implications for the Photocatalytic Reduction of CO₂. Energy & Fuels, 2009, 23, 5247-5256.	5.1	117
102	Quantum Mechanical Investigations of Heme Structure and Vibrational Spectra: Effects of Conformation, Oxidation State, and Electric Field. Langmuir, 2009, 25, 548-554.	3.5	8
103	Hydrogen Bonds and Vibrations of Water on (110) Rutile. Journal of Physical Chemistry C, 2009, 113, 13732-13740.	3.1	74
104	Density Functional Theory Study of Ferrihydrite and Related Fe-Oxyhydroxides. Chemistry of Materials, 2009, 21, 5727-5742.	6.7	81
105	Quantum chemical study of the Fe(III)-desferrioxamine B siderophore complexâ€"Electronic structure, vibrational frequencies, and equilibrium Fe-isotope fractionation. Geochimica Et Cosmochimica Acta, 2009, 73, 1-12.	3.9	67
106	Quantum Chemical Study of Arsenic (III, V) Adsorption on Mn-Oxides: Implications for Arsenic(III) Oxidation. Environmental Science & Technology, 2009, 43, 6655-6661.	10.0	154
107	Ferrous Iron Reduction of Superoxide, A Proton-Coupled Electron-Transfer Four-Point Test. Journal of Physical Chemistry A, 2009, 113, 1020-1025.	2.5	7
108	Origin of Nanoscale Phase Stability Reversals in Titanium Oxide Polymorphs. Journal of Physical Chemistry C, 2009, 113, 4240-4245.	3.1	62

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109	Reduction of N2 by Fe2+ via Homogeneous and Heterogeneous Reactions Part 2: The Role of Metal Binding in Activating N2 for Reduction; a Requirement for Both Pre-biotic and Biological Mechanisms. Origins of Life and Evolution of Biospheres, 2008, 38, 195-209.	1.9	10
110	Periodic density functional theory calculations of bulk and the (010) surface of goethite. Geochemical Transactions, 2008, 9, 4.	0.7	72
111	NMR spectroscopy of citrate in solids: crossâ€polarization kinetics in weakly coupled systems. Magnetic Resonance in Chemistry, 2008, 46, 408-417.	1.9	10
112	Transition State Theory and Molecular Orbital Calculations Applied to Rates and Reaction Mechanisms in Geochemical Kinetics. , 2008, , 39-72.		1
113	Density functional theory predictions of equilibrium isotope fractionation of iron due to redox changes and organic complexation. Geochimica Et Cosmochimica Acta, 2008, 72, 5201-5216.	3.9	72
114	Surface Protonation at the Rutile (110) Interface: Explicit Incorporation of Solvation Structure within the Refined MUSIC Model Framework. Langmuir, 2008, 24, 12331-12339.	3.5	88
115	Comparisons of Multilayer H₂O Adsorption onto the (110) Surfaces of Î±-TiO₂ and SnO₂ as Calculated with Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 11616-11624.	2.6	81
116	Quantum Chemical Modeling of Ground States of CO ₂ Chemisorbed on Anatase (001), (101), and (010) TiO ₂ Surfaces. Energy & Fuels, 2008, 22, 2611-2618.	5.1	59
117	The Mechanism Responsible for Extraordinary Cs Ion Selectivity in Crystalline Silicotitanate. Journal of the American Chemical Society, 2008, 130, 11689-11694.	13.7	132
118	Molecular modeling of Al3+ and benzene interactions with Suwannee fulvic acid. Geochimica Et Cosmochimica Acta, 2007, 71, 3859-3871.	3.9	10
119	Influence of Glycosidic Linkage Neighbors on Disaccharide Conformation in Vacuum. Journal of Physical Chemistry B, 2007, 111, 13775-13785.	2.6	19
120	Study of a Family of 40 Hydroxylated Î²-Cristobalite Surfaces Using Empirical Potential Energy Functions. Journal of Physical Chemistry C, 2007, 111, 5169-5177.	3.1	30
121	Calculating gas phase energies of an Î±(1â€“4) linked disaccharide: electronic structure theory and classical atomistic simulation. Computational and Theoretical Chemistry, 2007, 806, 9-22.	1.5	1
122	Surface complex structures modelled with quantum chemical calculations: carbonate, phosphate, sulphate, arsenate and arsenite. European Journal of Soil Science, 2007, 58, 932-944.	3.9	102
123	Sulphate adsorption at the Fe (hydr)oxide?H2O interface: comparison of cluster and periodic slab DFT predictions. European Journal of Soil Science, 2007, 58, 978-988.	3.9	49
124	Quantum Chemical Calculations of Sulfate Adsorption at the Al- and Fe-(Hydr)oxide-H2O InterfaceEstimation of Gibbs Free Energies. Environmental Science & Technology, 2006, 40, 7717-7724.	10.0	58
125	Model Bacterial Extracellular Polysaccharide Adsorption onto Silica and Alumina:Â Quartz Crystal Microbalance with Dissipation Monitoring of Dextran Adsorption. Environmental Science & Technology, 2006, 40, 7739-7744.	10.0	70
126	Derivation of Force Field Parameters for SnO2â^'H2O Surface Systems from Plane-Wave Density Functional Theory Calculations. Journal of Physical Chemistry B, 2006, 110, 8386-8397.	2.6	53

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127	Solid-State NMR and Computational Chemistry Study of Mononucleotides Adsorbed to Alumina. Langmuir, 2006, 22, 9281-9286.	3.5	46
128	Molecular Simulations of Benzene and PAH Interactions with Soot. Environmental Science & Technology, 2006, 40, 2298-2303.	10.0	46
129	Molecular Orbital Theory Study on Surface Complex Structures of Glyphosate on Goethite:â€‰ Calculation of Vibrational Frequencies. Environmental Science & Technology, 2006, 40, 3836-3841.	10.0	46
130	Silicate Glass and Mineral Dissolution:â€‰ Calculated Reaction Paths and Activation Energies for Hydrolysis of a Q3 Si by H3O+ Using Ab Initio Methods. Journal of Physical Chemistry A, 2006, 110, 198-206.	2.5	134
131	Deprotonation energies of a model fulvic acid. I. Carboxylic acid groups. Geochimica Et Cosmochimica Acta, 2006, 70, 44-55.	3.9	21
132	Interactions of biopolymers with silica surfaces: Force measurements and electronic structure calculation studies. Geochimica Et Cosmochimica Acta, 2006, 70, 3803-3819.	3.9	35
133	Structure of hydrated Zn2+ at the rutile TiO2 (110)-aqueous solution interface: Comparison of X-ray standing wave, X-ray absorption spectroscopy, and density functional theory results. Geochimica Et Cosmochimica Acta, 2006, 70, 4039-4056.	3.9	52
134	The role of structured water in the calibration and interpretation of theoretical IR spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 324-332.	3.9	2
135	Correlation of observed and model vibrational frequencies for aqueous organic acids: UV resonance Raman spectra and molecular orbital calculations of benzoic, salicylic, and phthalic acids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 2622-2633.	3.9	13
136	Sorption of the antibiotic ofloxacin to mesoporous and nonporous alumina and silica. Journal of Colloid and Interface Science, 2005, 283, 160-170.	9.4	173
137	Second-harmonic generation and theoretical studies of protonation at the water/Î±-TiO2 (110) interface. Chemical Physics Letters, 2005, 411, 399-403.	2.6	81
138	Computational chemistry applied to studies of organic contaminants in the environment: Examples based on benzo[a]pyrene. Numerische Mathematik, 2005, 305, 621-644.	1.4	11
139	Comparison of As(III) and As(V) Complexation onto Al- and Fe-Hydroxides. ACS Symposium Series, 2005, , 104-117.	0.5	21
140	Effect of Dehydration on Sulfate Coordination and Speciation at the Feâˆ'(Hydr)oxideâˆ'Water Interface:Â A Molecular Orbital/Density Functional Theory and Fourier Transform Infrared Spectroscopic Investigation. Langmuir, 2005, 21, 11071-11078.	3.5	64
141	ATR-FTIR spectroscopic characterization of coexisting carbonate surface complexes on hematite. Geochimica Et Cosmochimica Acta, 2005, 69, 1527-1542.	3.9	166
142	Theoretical and 27Al CPMAS NMR investigation of aluminum coordination changes during aluminosilicate dissolution. Geochimica Et Cosmochimica Acta, 2005, 69, 2205-2220.	3.9	72
143	A mechanism for carbon isotope exchange between aqueous acetic acid and : An ab initio study. Organic Geochemistry, 2005, 36, 835-850.	1.8	11
144	Mechanism of Hydroxyl Radical Generation from a Silica Surface:Â Molecular Orbital Calculations. Journal of Physical Chemistry B, 2005, 109, 21796-21807.	2.6	67

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145	Mechanistic Aspects of Pyrite Oxidation in an Oxidizing Gaseous Environment:Â An in Situ HATRâˆ'IR Isotope Study. Environmental Science & Technology, 2005, 39, 7576-7584.	10.0	43
146	Adhesion of Bacterial Exopolymers to Î±-FeOOH:Â Inner-Sphere Complexation of Phosphodiester Groups. Langmuir, 2004, 20, 11108-11114.	3.5	122
147	UV Resonance Raman Spectra and Molecular Orbital Calculations of Salicylic and Phthalic Acids Complexed to Al3+ in Solution and on Mineral Surfaces. Journal of Physical Chemistry A, 2004, 108, 11580-11590.	2.5	17
148	Adsorption of Water on the TiO2(Rutile) (110) Surface:Â A Comparison of Periodic and Embedded Cluster Calculations. Journal of Physical Chemistry B, 2004, 108, 7844-7853.	2.6	126
149	Electric Double Layer at the Rutile (110) Surface. 1. Structure of Surfaces and Interfacial Water from Molecular Dynamics by Use of ab Initio Potentials. Journal of Physical Chemistry B, 2004, 108, 12049-12060.	2.6	272
150	Ion Adsorption at the Rutileâˆ'Water Interface:Â Linking Molecular and Macroscopic Properties. Langmuir, 2004, 20, 4954-4969.	3.5	298
151	Oxygen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. Geochimica Et Cosmochimica Acta, 2004, 68, 949-958.	3.9	13
152	Ab initio calculation of 1H, 17O, 27Al and 29Si NMR parameters, vibrational frequencies and bonding energetics in hydrous silica and Na-aluminosilicate glasses. Geochimica Et Cosmochimica Acta, 2004, 68, 3909-3918.	3.9	27
153	Molecular Orbital Theory Study on Surface Complex Structures of Phosphates to Iron Hydroxides:Â Calculation of Vibrational Frequencies and Adsorption Energies. Langmuir, 2004, 20, 9249-9254.	3.5	152
154	High Temperature Microelectrophoresis Studies of the Rutile/Aqueous Solution Interface. Langmuir, 2003, 19, 3797-3804.	3.5	52
155	Derivation of Force Field Parameters for TiO2âˆ'H2O Systems from ab Initio Calculations. Journal of Physical Chemistry B, 2003, 107, 11072-11081.	2.6	196
156	Hydrogen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. Geochimica Et Cosmochimica Acta, 2003, 67, 1259-1276.	3.9	20
157	Molecular orbital modeling of aqueous organosilicon complexes: implications for silica biomineralization. Geochimica Et Cosmochimica Acta, 2003, 67, 4113-4121.	3.9	37
158	Molecular Modeling of Fulvic and Humic Acids. , 2003, , .		1
159	Dissolved organic carbon--contaminant interaction descriptors found by 3D force field calculations. SAR and QSAR in Environmental Research, 2002, 13, 271-280.	2.2	4
160	Molecular orbital calculations on aluminosilicate tricluster molecules: Implications for the structure of aluminosilicate glasses. American Mineralogist, 2002, 87, 668-678.	1.9	66
161	Characterisation of gallium(iii)-acetate complexes in aqueous solution: A potentiometric, EXAFS, IR and molecular orbital modelling study. Dalton Transactions RSC, 2002, , 2559-2564.	2.3	19
162	Self-Consistent Reaction Field Calculations of Aqueous Al3+, Fe3+, and Si4+:â€‰ Calculated Aqueous-Phase Deprotonation Energies Correlated with Experimental ln(Ka) and pKa. Journal of Physical Chemistry A, 2001, 105, 8756-8762.	2.5	58

#	Article	IF	Citations
163	Dissolution of nepheline, jadeite and albite glasses: toward better models for aluminosilicate dissolution. Geochimica Et Cosmochimica Acta, 2001, 65, 3683-3702.	3.9	180
164	13. Interpretation of Vibrational Spectra Using Molecular Orbital Theory Calculations. , 2001, , 459-484.		5
165	Molecular Orbital Modeling and Transition State Theory in Geochemistry. Reviews in Mineralogy and Geochemistry, 2001, 42, 485-531.	4.8	12
166	Interpretation of Vibrational Spectra Using Molecular Orbital Theory Calculations. Reviews in Mineralogy and Geochemistry, 2001, 42, 459-483.	4.8	17
167	Gas-Phase Acidities of Tetrahedral Oxyacids from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2000, 104, 4051-4057.	2.5	41
168	Molecular models of benzene and selected polycyclic aromatic hydrocarbons in the aqueous and adsorbed states. Environmental Toxicology and Chemistry, 1999, 18, 1656-1662.	4.3	16
169	Models of natural organic matter and interactions with organic contaminants. Organic Geochemistry, 1999, 30, 911-927.	1.8	88
170	Attenuated total reflectance Fourier-transform infrared spectroscopy of carboxylic acids adsorbed onto mineral surfaces. Geochimica Et Cosmochimica Acta, 1999, 63, 2709-2725.	3.9	195
171	Ab Initio Calculation of Aqueous Aluminum and Aluminumâˆ'Carboxylate Complex Energetics and 27Al NMR Chemical Shifts. Journal of Physical Chemistry A, 1999, 103, 903-915.	2.5	82
172	MOLECULAR MODELS OF BENZENE AND SELECTED POLYCYCLIC AROMATIC HYDROCARBONS IN THE AQUEOUS AND ADSORBED STATES. Environmental Toxicology and Chemistry, 1999, 18, 1656.	4.3	2
173	Molecular cluster models of aluminum oxide and aluminum hydroxide surfaces. American Mineralogist, 1998, 83, 1054-1066.	1.9	54
174	Bonding Mechanisms of Salicylic Acid Adsorbed onto Illite Clay:Â An ATRâˆ'FTIR and Molecular Orbital Study. Environmental Science & Technology, 1997, 31, 1151-1156.	10.0	101
175	Molecular Orbital Calculation of27Al and29Si NMR Parameters in Q3and Q4Aluminosilicate Molecules and Implications for the Interpretation of Hydrous Aluminosilicate Glass NMR Spectra. Journal of Physical Chemistry A, 1997, 101, 2715-2722.	2.5	62
176	Molecular orbital calculations for modeling acetate-aluminosilicate adsorption and dissolution reactions. Geochimica Et Cosmochimica Acta, 1997, 61, 1031-1046.	3.9	34
177	Molecular orbital models of aqueous aluminum-acetate complexes. Geochimica Et Cosmochimica Acta, 1996, 60, 4897-4911.	3.9	48
178	Four-membered rings in silica and aluminosilicate glasses. American Mineralogist, 1996, 81, 265-272.	1.9	58
179	Structural roles of CO2 and [CO3]2âˆ' in fully polymerized sodium aluminosilicate melts and glasses. Geochimica Et Cosmochimica Acta, 1995, 59, 683-698.	3.9	41
180	Molecular orbital calculations on the vibrational spectra of Q3 T-(OH) species and the hydrolysis of a three-membered aluminosilicate ring. Geochimica Et Cosmochimica Acta, 1995, 59, 4791-4797.	3.9	28

#	Article	IF	Citations
181	â€œTheoretical reaction pathways for the formation of [Si(OH)5]1- and the deprotonation of orthosilicicacid in basic solution.â€•Geochimica et Cosmochimica Acta. Geochimica Et Cosmochimica Acta, 1994, 58, 2755-2756.	3.9	2
182	Reply to the comment by S.C. Kohn, M.E. Smith, and R. Dupree on â€œA model for H2O solubility mechanisms in albite melts from infrared spectroscopy and molecular orbital calculationsâ€• Geochimica Et Cosmochimica Acta, 1994, 58, 1381-1384.	3.9	27
183	Calculated trends of oh infrared stretching vibrations with composition and structure in aluminosilicate molecules. Physics and Chemistry of Minerals, 1993, 20, 425.	0.8	37
184	Theoretical reaction pathways for the formation of [Si(OH)5]1âˆ’ and the deprotonation of orthosilicic acid in basic solution. Geochimica Et Cosmochimica Acta, 1993, 57, 3847-3853.	3.9	53
185	Molecular dynamics simulations of periclase crystallization. Geophysical Research Letters, 1993, 20, 2103-2106.	4.0	3
186	A model for H2O solubility mechanisms in albite melts from infrared spectroscopy and molecular orbital calculations. Geochimica Et Cosmochimica Acta, 1993, 57, 1039-1052.	3.9	95
187	Deep mantle melting. Nature, 1991, 349, 283-284.	27.8	5
188	Chemical diffusion in melts on the CaMgSi2O6-CaAl2Si2O8 join under high pressures. Geochimica Et Cosmochimica Acta, 1990, 54, 2709-2715.	3.9	27