James D Kubicki

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

192 papers	8,322 citations	53 h-index	82 g-index
206 ext. papers	9,092 ext. citations	5.1 avg, IF	6.19 L-index

#	Paper	IF	Citations
192	Density Functional Tight-Binding Simulations Reveal the Presence of Surface Defects on the Quartz (101)Water Interface. *Journal of Physical Chemistry C*, **2021**, 125, 16246-16255	3.8	
191	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	5.5	3
190	In silico structure prediction of full-length cotton cellulose synthase protein (GhCESA1) and its hierarchical complexes. *Cellulose*, **2020**, 27, 5597-5616	5.5	3
189	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	5.5	14
188	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	4	6
187	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	3.5	4
186	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	3.2	1
185	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	2.8	3
184	Probing cellulose structures with vibrational spectroscopy. *Cellulose*, **2019**, 26, 35-79	5.5	60
183	Quantum Mechanical Modeling of the Vibrational Spectra of Minerals with a Focus on Clays. *Minerals (Basel, Switzerland)*, **2019**, 9, 141	2.4	15
182	Simulations of Cellulose Synthesis Initiation and Termination in Bacteria. *Journal of Physical Chemistry B*, **2019**, 123, 3699-3705	3.4	8
181	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	3.2	8
180	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	2.8	5
179	Evaluating Computational Chemistry Methods for Isotopic Fractionation between CO(g) and HO(g). *Journal of Chemical Information and Modeling*, **2019**, 59, 4663-4677	6.1	1
178	Integrating Density Functional Theory Calculations with Vibrational and Nuclear Magnetic Resonance Spectroscopy. *ACS Symposium Series*, **2019**, 89-102	0.4	
177	Simultaneous Adsorption and Incorporation of Sr2+ at the Barite (001)Water Interface. *Journal of Physical Chemistry C*, **2019**, 123, 1194-1207	3.8	10
176	Arabinose substitution effect on xylan rigidity and self-aggregation. *Cellulose*, **2019**, 26, 2267-2278	5.5	17

175	Quantum Calculations on Plant Cell Wall Component Interactions. *Interdisciplinary Sciences, Computational Life Sciences*, **2019**, 11, 485-495	3.5	8
174	Initiation, Elongation, and Termination of Bacterial Cellulose Synthesis. *ACS Omega*, **2018**, 3, 2690-2698	3.9	13
173	An evaluation of the structures of cellulose generated by the CHARMM force field: comparisons to in planta cellulose. *Cellulose*, **2018**, 25, 3755-3777	5.5	11
172	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	5.5	22
171	Binding Geometries of Silicate Species on Ferrihydrite Surfaces. *ACS Earth and Space Chemistry*, **2018**, 2, 125-134	3.2	25
170	Density functional theory modeling of chromate adsorption onto ferrihydrite nanoparticles. *Geochemical Transactions*, **2018**, 19, 8	3	19
169	Structural factors affecting 13C NMR chemical shifts of cellulose: a computational study. *Cellulose*, **2018**, 25, 23-36	5.5	35
168	Reaction Mechanisms and Solid□as Phase Reactions: Theory and Density Functional Theory Simulations. *Reviews in Mineralogy and Geochemistry*, **2018**, 84, 85-101	7.1	4
167	3. Reaction Mechanisms and Solid□as Phase Reactions: Theory and Density Functional Theory Simulations **2018**, 85-102		
166	The Shape of Native Plant Cellulose Microfibrils. *Scientific Reports*, **2018**, 8, 13983	4.9	47
165	Kinetic analysis of cellulose synthase of Gluconacetobacter hansenii in whole cells and in purified form. *Enzyme and Microbial Technology*, **2018**, 119, 24-29	3.8	1
164	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	4.2	19
163	Fourier-transform infrared spectroscopy (FTIR) analysis of triclinic and hexagonal birnessites. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2017**, 178, 32-46	4.4	27
162	Interactions between aromatic hydrocarbons and functionalized C60 fullerenes □nsights from experimental data and molecular modelling. *Environmental Science: Nano*, **2017**, 4, 1045-1053	7.1	15
161	Effect of amino acids on the precipitation kinetics and Ca isotopic composition of gypsum. *Geochimica Et Cosmochimica Acta*, **2017**, 218, 343-364	5.5	14
160	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	4.2	30
159	Competitive Adsorption of Acetic Acid and Water on Kaolinite. *Journal of Physical Chemistry A*, **2016** , 120, 8339-8346	2.8	11
158	Effect of Ions on H-Bond Structure and Dynamics at the Quartz(101)-Water Interface. *Langmuir*, **2016**, 32, 11353-11365	4	31

157	Sustainable development of a surface-functionalized mesoporous aluminosilicate with ultra-high ion exchange efficiency. *Inorganic Chemistry Frontiers*, **2016**, 3, 502-513	6.8	17
156	X-ray Absorption Spectroscopic Quantification and Speciation Modeling of Sulfate Adsorption on Ferrihydrite Surfaces. *Environmental Science & Technology*, **2016**, 50, 8067-76	10.3	73
155	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, 2210-22	6.9	68
154	Spectroscopy and Ultrafast Vibrational Dynamics of Strongly Hydrogen Bonded OH Species at the □Al2O3(112 0)/H2O Interface. *Journal of Physical Chemistry C*, **2016**, 120, 16153-16161	3.8	33
153	Vibrational Spectroscopy of Minerals Through Ab Initio Methods **2016**, 341-374		1
152	Geochemical Kinetics via Computational Chemistry **2016**, 375-414		1
151	Force Field Application and Development **2016**, 33-75		2
150	First Principles Estimation of Geochemically Important Transition Metal Oxide Properties **2016**, 107-149		6
149	Computational Isotope Geochemistry **2016**, 151-175		2
148	Organic and Contaminant Geochemistry **2016**, 177-243		3
147	Petroleum Geochemistry **2016**, 245-269		
146	Mineral□Water Interaction **2016**, 271-309		5
145	How Cellulose Elongates--A QM/MM Study of the Molecular Mechanism of Cellulose Polymerization in Bacterial CESA. *Journal of Physical Chemistry B*, **2015**, 119, 6525-35	3.4	12
144	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, 15138-49	3.4	111
143	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, 703-13	4	8
142	Rb+ Adsorption at the Quartz(101)□Aqueous Interface: Comparison of Resonant Anomalous X-ray Reflectivity with ab Initio Calculations. *Journal of Physical Chemistry C*, **2015**, 119, 4778-4788	3.8	26
141	Plagioclase dissolution during CO□SO□cosequestration: effects of sulfate. *Environmental Science & Technology*, **2015**, 49, 1946-54	10.3	19
140	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	5.5	20

139	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	3.8	43
138	Stereochemistry, elution order and molecular modeling of four diaergostanes in petroleum. *Organic Geochemistry*, **2014**, 76, 1-8	3.1	7
137	Towards lignin-protein crosslinking: amino acid adducts of a lignin model quinone methide. *Cellulose*, **2014**, 21, 1395-1407	5.5	7
136	Molecular dynamics simulation study of xyloglucan adsorption on cellulose surfaces: effects of surface hydrophobicity and side-chain variation. *Cellulose*, **2014**, 21, 1025-1039	5.5	69
135	Constraints on ({rm I}beta) cellulose twist from DFT calculations of (^{13}hbox {C}) NMR chemical shifts. *Cellulose*, **2014**, 21, 3979-3991	5.5	13
134	Quantum mechanical modeling of hydrolysis and H2O-exchange in Mg-, Ca-, and Nisilicate clusters: Implications for dissolution mechanisms of olivine minerals. *American Mineralogist*, **2014**, 99, 2303-2312	2.9	10
133	Arsenic Adsorption onto Minerals: Connecting Experimental Observations with Density Functional Theory Calculations. *Minerals (Basel, Switzerland)*, **2014**, 4, 208-240	2.4	47
132	Quantum mechanical calculations on cellulose□water interactions: structures, energetics, vibrational frequencies and NMR chemical shifts for surfaces of I□and I□cellulose. *Cellulose*, **2014**, 21, 909-926	5.5	25
131	Molecular level investigations of phosphate sorption on corundum (□Al2O3) by 31P solid state NMR, ATR-FTIR and quantum chemical calculation. *Geochimica Et Cosmochimica Acta*, **2013**, 107, 252-266	5.5	74
130	Adsorption of carbon dioxide on Al/Fe oxyhydroxide. *Journal of Colloid and Interface Science*, **2013**, 400, 1-10	9.3	17
129	Cellulose microfibril twist, mechanics, and implication for cellulose biosynthesis. *Journal of Physical Chemistry A*, **2013**, 117, 2580-9	2.8	67
128	Development of a ReaxFF reactive force field for titanium dioxide/water systems. *Langmuir*, **2013**, 29, 7838-46	4	77
127	In situ structural characterization of ferric iron dimers in aqueous solutions: identification of □xo species. *Inorganic Chemistry*, **2013**, 52, 6788-97	5.1	33
126	Sum-frequency-generation vibration spectroscopy and density functional theory calculations with dispersion corrections (DFT-D2) for cellulose I□and I□*Journal of Physical Chemistry B*, **2013**, 117, 6681-92	3.4	79
125	Anatase nanoparticle surface reactivity in NaCl media: a CD-MUSIC model interpretation of combined experimental and density functional theory studies. *Langmuir*, **2013**, 29, 8572-83	4	8
124	Identification and characterization of a cellulose binding heptapeptide revealed by phage display. *Biomacromolecules*, **2013**, 14, 1795-805	6.9	27
123	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	3.8	16
122	Quantum mechanical modeling of the structures, energetics and spectral properties of I□and I□ cellulose. *Cellulose*, **2013**, 20, 9-23	5.5	36

121	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	3.8	31
120	Tertiary model of a plant cellulose synthase. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 7512-7	11.5	129
119	Molecular dynamics simulations of the interactions between TiO2 nanoparticles and water with Na+ and Cl methanol, and formic acid using a reactive force field. *Journal of Materials Research*, **2013**, 28, 513-520	2.5	44
118	ATR-FTIR and density functional theory study of the structures, energetics, and vibrational spectra of phosphate adsorbed onto goethite. *Langmuir*, **2012**, 28, 14573-87	4	105
117	Comment on Structure and dynamics of liquid water on rutile TiO2(110) *Physical Review B*, **2012**, 85,	3.3	42
116	Quantum mechanical calculations on FeOH nanoparticles. *Geoderma*, **2012**, 189-190, 236-242	6.7	9
115	A New Hypothesis for the Dissolution Mechanism of Silicates. *Journal of Physical Chemistry C*, **2012**, 116, 17479-17491	3.8	44
114	Molecular models of birnessite and related hydrated layered minerals. *American Mineralogist*, **2012**, 97, 1505-1514	2.9	29
113	In search of OH 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	3.4	5
112	Adsorption of nitrate on kaolinite surfaces: a theoretical study. *Journal of Physical Chemistry B*, **2012**, 116, 11266-73	3.4	17
111	Aluminum coprecipitates with Fe (hydr)oxides: Does isomorphous substitution of Al3+ for Fe3+ in goethite occur?. *Geochimica Et Cosmochimica Acta*, **2011**, 75, 4667-4683	5.5	43
110	Simulations of the Quartz(101 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	3.8	145
109	Periodic Density Functional Theory Study of Water Adsorption on the Quartz (101) Surface. *Journal of Physical Chemistry C*, **2011**, 115, 5756-5766	3.8	59
108	Faster proton transfer dynamics of water on SnO2 compared to TiO2. *Journal of Chemical Physics*, **2011**, 134, 044706	3.9	32
107	Electronic structure, chemical bonding, and oxidation numbers of first-row transition metals in [MePIm2] complexes and their cations. *International Journal of Quantum Chemistry*, **2011**, 111, 3630-3642	2.1	1
106	Evaluation of potential reaction mechanisms leading to the formation of coniferyl alcohol linkages in lignin: a density functional theory study. *Physical Chemistry Chemical Physics*, **2011**, 13, 20974-85	3.6	12
105	Evaluating glutamate and aspartate binding mechanisms to rutile (TiO2) via ATR-FTIR spectroscopy and quantum chemical calculations. *Langmuir*, **2011**, 27, 1778-87	4	53
104	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	3.8	9

103	Differential pair distribution function study of the structure of arsenate adsorbed on nanocrystalline □alumina. *Environmental Science & Technology*, **2011**, 45, 9687-92	10.3	58
102	Comparison of cation adsorption by isostructural rutile and cassiterite. *Langmuir*, **2011**, 27, 4585-93	4	25
101	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, 1958-70	3.4	36
100	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	42
99	Description of Mg2+ Release from Forsterite Using Ab Initio Methods□ *Journal of Physical Chemistry C*, **2010**, 114, 5417-5428	3.8	15
98	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	4.2	6
97	Development of a reactive force field for iron-oxyhydroxide systems. *Journal of Physical Chemistry A*, **2010**, 114, 6298-307	2.8	145
96	Surface speciation of phosphate on boehmite (gamma-AlOOH) determined from NMR spectroscopy. *Langmuir*, **2010**, 26, 4753-61	4	54
95	Photodissolution of ferrihydrite in the presence of oxalic acid: an in situ ATR-FTIR/DFT study. *Langmuir*, **2010**, 26, 16246-53	4	42
94	Interaction energy and the shift in OH stretch frequency on hydrogen bonding for the H2O --> H2O, CH3OH --> H2O, and H2O --> CH3OH dimers. *Journal of Computational Chemistry*, **2010**, 31, 963-72	3.5	11
93	Computational Spectroscopy in Environmental Chemistry **2010**, 323-351		2
92	Reductive dissolution of ferrihydrite by ascorbic acid and the inhibiting effect of phospholipid. *Journal of Colloid and Interface Science*, **2010**, 341, 215-23	9.3	19
91	Surface science studies of environmentally relevant iron (oxy)hydroxides ranging from the nano to the macro-regime. *Surface Science*, **2010**, 604, 1065-1071	1.8	5
90	MP2, density functional theory, and molecular mechanical calculations of C-H...pi and hydrogen bond interactions in a cellulose-binding module-cellulose model system. *Carbohydrate Research*, **2010**, 345, 1741-51	2.9	30
89	Quantum mechanical calculation of aqueuous uranium complexes: carbonate, phosphate, organic and biomolecular species. *Chemistry Central Journal*, **2009**, 3, 10		57
88	Ferrihydrite reactivity toward carbon dioxide. *Journal of Colloid and Interface Science*, **2009**, 337, 492-500	9.3	59
87	Photoinduced activation of CO2 on Ti-based heterogeneous catalysts: Current state, chemical physics-based insights and outlook. *Energy and Environmental Science*, **2009**, 2, 745	35.4	578
86	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	4.1	108

85	Quantum mechanical investigations of heme structure and vibrational spectra: effects of conformation, oxidation state, and electric field. *Langmuir*, **2009**, 25, 548-54	4	8
84	Hydrogen Bonds and Vibrations of Water on (110) Rutile. *Journal of Physical Chemistry C*, **2009**, 113, 13732-13740	3.8	74
83	Density Functional Theory Study of Ferrihydrite and Related Fe-Oxyhydroxides. *Chemistry of Materials*, **2009**, 21, 5727-5742	9.6	66
82	Quantum chemical study of the Fe(III)-desferrioxamine B siderophore complex: Electronic structure, vibrational frequencies, and equilibrium Fe-isotope fractionation. *Geochimica Et Cosmochimica Acta*, **2009**, 73, 1-12	5.5	52
81	Quantum chemical study of arsenic (III, V) adsorption on Mn-oxides: implications for arsenic(III) oxidation. *Environmental Science & Technology*, **2009**, 43, 6655-61	10.3	132
80	Ferrous iron reduction of superoxide, a proton-coupled electron-transfer four-point test. *Journal of Physical Chemistry A*, **2009**, 113, 1020-5	2.8	7
79	Origin of Nanoscale Phase Stability Reversals in Titanium Oxide Polymorphs. *Journal of Physical Chemistry C*, **2009**, 113, 4240-4245	3.8	58
78	Transition State Theory and Molecular Orbital Calculations Applied to Rates and Reaction Mechanisms in Geochemical Kinetics **2008**, 39-72		1
77	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	5.5	56
76	Surface protonation at the rutile (110) interface: explicit incorporation of solvation structure within the refined MUSIC model framework. *Langmuir*, **2008**, 24, 12331-9	4	84
75	Comparisons of multilayer H2O adsorption onto the (110) surfaces of alpha-TiO2 and SnO2 as calculated with density functional theory. *Journal of Physical Chemistry B*, **2008**, 112, 11616-24	3.4	74
74	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	4.1	53
73	The mechanism responsible for extraordinary Cs ion selectivity in crystalline silicotitanate. *Journal of the American Chemical Society*, **2008**, 130, 11689-94	16.4	115
72	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	1.5	7
71	Periodic density functional theory calculations of bulk and the (010) surface of goethite. *Geochemical Transactions*, **2008**, 9, 4	3	66
70	NMR spectroscopy of citrate in solids: cross-polarization kinetics in weakly coupled systems. *Magnetic Resonance in Chemistry*, **2008**, 46, 408-17	2.1	9
69	Influence of glycosidic linkage neighbors on disaccharide conformation in vacuum. *Journal of Physical Chemistry B*, **2007**, 111, 13775-85	3.4	19
68	Study of a Family of 40 Hydroxylated Cristobalite Surfaces Using Empirical Potential Energy Functions. *Journal of Physical Chemistry C*, **2007**, 111, 5169-5177	3.8	27

67	Calculating gas phase energies of an (1→4) linked disaccharide: electronic structure theory and classical atomistic simulation. *Computational and Theoretical Chemistry*, **2007**, 806, 9-22		1
66	Surface complex structures modelled with quantum chemical calculations: carbonate, phosphate, sulphate, arsenate and arsenite. *European Journal of Soil Science*, **2007**, 58, 932-944	3.4	87
65	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	3.4	42
64	Molecular modeling of Al3+ and benzene interactions with Suwannee fulvic acid. *Geochimica Et Cosmochimica Acta*, **2007**, 71, 3859-3871	5.5	10
63	Quantum chemical calculations of sulfate adsorption at the Al- and Fe-(hydr)oxide-H20 interface-estimation of gibbs free energies. *Environmental Science & Technology*, **2006**, 40, 7717-24	10.3	58
62	Model bacterial extracellular polysaccharide adsorption onto silica and alumina: quartz crystal microbalance with dissipation monitoring of dextran adsorption. *Environmental Science & Technology*, **2006**, 40, 7739-44	10.3	63
61	Derivation of force field parameters for SnO2-H2O surface systems from plane-wave density functional theory calculations. *Journal of Physical Chemistry B*, **2006**, 110, 8386-97	3.4	47
60	Solid-state NMR and computational chemistry study of mononucleotides adsorbed to alumina. *Langmuir*, **2006**, 22, 9281-6	4	33
59	Molecular simulations of benzene and PAH interactions with soot. *Environmental Science & Technology*, **2006**, 40, 2298-303	10.3	45
58	Molecular orbital theory study on surface complex structures of glyphosate on goethite: calculation of vibrational frequencies. *Environmental Science & Technology*, **2006**, 40, 3836-41	10.3	39
57	Silicate glass and mineral dissolution: 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	2.8	118
56	Deprotonation energies of a model fulvic acid. I. Carboxylic acid groups. *Geochimica Et Cosmochimica Acta*, **2006**, 70, 44-55	5.5	18
55	Interactions of biopolymers with silica surfaces: Force measurements and electronic structure calculation studies. *Geochimica Et Cosmochimica Acta*, **2006**, 70, 3803-3819	5.5	34
54	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	5.5	47
53	The role of structured water in the calibration and interpretation of theoretical IR spectra. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2006**, 65, 324-32	4.4	2
52	Effect of dehydration on sulfate coordination and speciation at the Fe-(hydr)oxide-water interface: a molecular orbital/density functional theory and Fourier transform infrared spectroscopic investigation. *Langmuir*, **2005**, 21, 11071-8	4	59
51	ATR-FTIR spectroscopic characterization of coexisting carbonate surface complexes on hematite. *Geochimica Et Cosmochimica Acta*, **2005**, 69, 1527-1542	5.5	144
50	Theoretical and 27Al CPMAS NMR investigation of aluminum coordination changes during aluminosilicate dissolution. *Geochimica Et Cosmochimica Acta*, **2005**, 69, 2205-2220	5.5	64

49	A mechanism for carbon isotope exchange between aqueous acetic acid and : An ab initio study. *Organic Geochemistry*, **2005**, 36, 835-850	3.1	10
48	Mechanism of hydroxyl radical generation from a silica surface: molecular orbital calculations. *Journal of Physical Chemistry B*, **2005**, 109, 21796-807	3.4	52
47	Mechanistic aspects of pyrite oxidation in an oxidizing gaseous environment: an in situ HATR-IR isotope study. *Environmental Science & Technology*, **2005**, 39, 7576-84	10.3	39
46	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, 2622-33	4.4	12
45	Sorption of the antibiotic ofloxacin to mesoporous and nonporous alumina and silica. *Journal of Colloid and Interface Science*, **2005**, 283, 160-70	9.3	144
44	Second-harmonic generation and theoretical studies of protonation at the water/TiO2 (110) interface. *Chemical Physics Letters*, **2005**, 411, 399-403	2.5	74
43	Computational chemistry applied to studies of organic contaminants in the environment: Examples based on benzo[a]pyrene. *Numerische Mathematik*, **2005**, 305, 621-644	5.3	11
42	Comparison of As(III) and As(V) Complexation onto Al- and Fe-Hydroxides. *ACS Symposium Series*, **2005**, 104-117	0.4	18
41	Adhesion of bacterial exopolymers to alpha-FeOOH: inner-sphere complexation of phosphodiester groups. *Langmuir*, **2004**, 20, 11108-14	4	107
40	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	2.8	17
39	Adsorption of Water on the TiO2(Rutile) (110) Surface:A Comparison of Periodic and Embedded Cluster Calculations. *Journal of Physical Chemistry B*, **2004**, 108, 7844-7853	3.4	122
38	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	3.4	245
37	Ion adsorption at the rutile-water interface: linking molecular and macroscopic properties. *Langmuir*, **2004**, 20, 4954-69	4	280
36	Oxygen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. *Geochimica Et Cosmochimica Acta*, **2004**, 68, 949-958	5.5	11
35	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	5.5	23
34	Molecular orbital theory study on surface complex structures of phosphates to iron hydroxides: calculation of vibrational frequencies and adsorption energies. *Langmuir*, **2004**, 20, 9249-54	4	130
33	High Temperature Microelectrophoresis Studies of the Rutile/Aqueous Solution Interface. *Langmuir*, **2003**, 19, 3797-3804	4	48
32	Derivation of Force Field Parameters for TiO2H2O Systems from ab Initio Calculations. *Journal of Physical Chemistry B*, **2003**, 107, 11072-11081	3.4	177

31	Hydrogen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. *Geochimica Et Cosmochimica Acta*, **2003**, 67, 1259-1276	5.5	17
30	Molecular orbital modeling of aqueous organosilicon complexes: implications for silica biomineralization. *Geochimica Et Cosmochimica Acta*, **2003**, 67, 4113-4121	5.5	32
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