James D Kubicki

List of Publications by Citations

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	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
191	Ion adsorption at the rutile-water interface: linking molecular and macroscopic properties. *Langmuir*, **2004**, 20, 4954-69	4	280
190	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
189	Derivation of Force Field Parameters for TiO2H2O Systems from ab Initio Calculations. *Journal of Physical Chemistry B*, **2003**, 107, 11072-11081	3.4	177
188	Attenuated total reflectance Fourier-transform infrared spectroscopy of carboxylic acids adsorbed onto mineral surfaces. *Geochimica Et Cosmochimica Acta*, **1999**, 63, 2709-2725	5.5	171
187	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
186	Development of a reactive force field for iron-oxyhydroxide systems. *Journal of Physical Chemistry A*, **2010**, 114, 6298-307	2.8	145
185	Dissolution of nepheline, jadeite and albite glasses: toward better models for aluminosilicate dissolution. *Geochimica Et Cosmochimica Acta*, **2001**, 65, 3683-3702	5.5	145
184	ATR-FTIR spectroscopic characterization of coexisting carbonate surface complexes on hematite. *Geochimica Et Cosmochimica Acta*, **2005**, 69, 1527-1542	5.5	144
183	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
182	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
181	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
180	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
179	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
178	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
177	The mechanism responsible for extraordinary Cs ion selectivity in crystalline silicotitanate. *Journal of the American Chemical Society*, **2008**, 130, 11689-94	16.4	115
176	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

175	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
174	Adhesion of bacterial exopolymers to alpha-FeOOH: inner-sphere complexation of phosphodiester groups. *Langmuir*, **2004**, 20, 11108-14	4	107
173	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
172	Bonding Mechanisms of Salicylic Acid Adsorbed onto Illite Clay:An ATRFTIR and Molecular Orbital Study. *Environmental Science & Technology*, **1997**, 31, 1151-1156	10.3	93
171	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
170	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
169	A model for H2O solubility mechanisms in albite melts from infrared spectroscopy and molecular orbital calculations. *Geochimica Et Cosmochimica Acta*, **1993**, 57, 1039-1052	5.5	81
168	Models of natural organic matter and interactions with organic contaminants. *Organic Geochemistry* , **1999**, 30, 911-927	3.1	80
167	Sum-frequency-generation vibration spectroscopy and density functional theory calculations with dispersion corrections (DFT-D2) for cellulose Iand I*Journal of Physical Chemistry B*, **2013**, 117, 6681-92	3.4	79
166	Development of a ReaxFF reactive force field for titanium dioxide/water systems. *Langmuir*, **2013**, 29, 7838-46	4	77
165	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
164	Hydrogen Bonds and Vibrations of Water on (110) Rutile. *Journal of Physical Chemistry C*, **2009**, 113, 13732-13740	3.2	74
163	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
162	Second-harmonic generation and theoretical studies of protonation at the water/TiO2 (110) interface. *Chemical Physics Letters*, **2005**, 411, 399-403	2.5	74
161	Ab Initio Calculation of Aqueous Aluminum and Aluminumcarboxylate Complex Energetics and 27Al NMR Chemical Shifts. *Journal of Physical Chemistry A*, **1999**, 103, 903-915	2.8	74
160	X-ray Absorption Spectroscopic Quantification and Speciation Modeling of Sulfate Adsorption on Ferrihydrite Surfaces. *Environmental Science & Technology*, **2016**, 50, 8067-76	10.3	73
159	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
158	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

157	Cellulose microfibril twist, mechanics, and implication for cellulose biosynthesis. *Journal of Physical Chemistry A*, **2013**, 117, 2580-9	2.8	67
156	Density Functional Theory Study of Ferrihydrite and Related Fe-Oxyhydroxides. *Chemistry of Materials*, **2009**, 21, 5727-5742	9.6	66
155	Periodic density functional theory calculations of bulk and the (010) surface of goethite. *Geochemical Transactions*, **2008**, 9, 4	3	66
154	Theoretical and 27Al CPMAS NMR investigation of aluminum coordination changes during aluminosilicate dissolution. *Geochimica Et Cosmochimica Acta*, **2005**, 69, 2205-2220	5.5	64
153	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
152	Probing cellulose structures with vibrational spectroscopy. *Cellulose*, **2019**, 26, 35-79	5.5	60
151	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
150	Ferrihydrite reactivity toward carbon dioxide. *Journal of Colloid and Interface Science*, **2009**, 337, 492-500	9.3	59
149	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
148	Differential pair distribution function study of the structure of arsenate adsorbed on nanocrystalline □alumina. *Environmental Science & Technology*, **2011**, 45, 9687-92	10.3	58
147	Origin of Nanoscale Phase Stability Reversals in Titanium Oxide Polymorphs. *Journal of Physical Chemistry C*, **2009**, 113, 4240-4245	3.8	58
146	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
145	Quantum mechanical calculation of aqueuous uranium complexes: carbonate, phosphate, organic and biomolecular species. *Chemistry Central Journal*, **2009**, 3, 10		57
144	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
143	Molecular orbital calculations on aluminosilicate tricluster molecules: Implications for the structure of aluminosilicate glasses. *American Mineralogist*, **2002**, 87, 668-678	2.9	56
142	Self-Consistent Reaction Field Calculations of Aqueous Al3+, Fe3+, and Si4+: Calculated Aqueous-Phase Deprotonation Energies Correlated with Experimental ln(Ka) and pKa. *Journal of Physical Chemistry A*, **2001**, 105, 8756-8762	2.8	55
141	Surface speciation of phosphate on boehmite (gamma-AlOOH) determined from NMR spectroscopy. *Langmuir*, **2010**, 26, 4753-61	4	54
140	Evaluating glutamate and aspartate binding mechanisms to rutile (□TiO2) via ATR-FTIR spectroscopy and quantum chemical calculations. *Langmuir*, **2011**, 27, 1778-87	4	53

139	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
138	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
137	Mechanism of hydroxyl radical generation from a silica surface: molecular orbital calculations. *Journal of Physical Chemistry B*, **2005**, 109, 21796-807	3.4	52
136	Molecular Orbital Calculation of 27Al and 29Si NMR Parameters in Q3 and Q4 Aluminosilicate Molecules and Implications for the Interpretation of Hydrous Aluminosilicate Glass NMR Spectra. *Journal of Physical Chemistry A*, **1997**, 101, 2715-2722	2.8	51
135	High Temperature Microelectrophoresis Studies of the Rutile/Aqueous Solution Interface. *Langmuir*, **2003**, 19, 3797-3804	4	48
134	Arsenic Adsorption onto Minerals: Connecting Experimental Observations with Density Functional Theory Calculations. *Minerals (Basel, Switzerland)*, **2014**, 4, 208-240	2.4	47
133	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
132	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
131	Theoretical reaction pathways for the formation of [Si(OH)5]1 and the deprotonation of orthosilicic acid in basic solution. *Geochimica Et Cosmochimica Acta*, **1993**, 57, 3847-3853	5.5	47
130	The Shape of Native Plant Cellulose Microfibrils. *Scientific Reports*, **2018**, 8, 13983	4.9	47
129	Molecular simulations of benzene and PAH interactions with soot. *Environmental Science & Technology*, **2006**, 40, 2298-303	10.3	45
128	Four-membered rings in silica and aluminosilicate glasses. *American Mineralogist*, **1996**, 81, 265-272	2.9	45
127	A New Hypothesis for the Dissolution Mechanism of Silicates. *Journal of Physical Chemistry C*, **2012**, 116, 17479-17491	3.8	44
126	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
125	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
124	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
123	Molecular cluster models of aluminum oxide and aluminum hydroxide surfaces. *American Mineralogist*, **1998**, 83, 1054-1066	2.9	43
122	Molecular orbital models of aqueous aluminum-acetate complexes. *Geochimica Et Cosmochimica Acta*, **1996**, 60, 4897-4911	5.5	43

121	Comment on Structure and dynamics of liquid water on rutile TiO2(110) *Physical Review B*, **2012**, 85,	3.3	42
120	Photodissolution of ferrihydrite in the presence of oxalic acid: an in situ ATR-FTIR/DFT study. *Langmuir*, **2010**, 26, 16246-53	4	42
119	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
118	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
117	Gas-Phase Acidities of Tetrahedral Oxyacids from ab Initio Electronic Structure Theory. *Journal of Physical Chemistry A*, **2000**, 104, 4051-4057	2.8	40
116	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
115	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
114	Structural roles of CO2 and [CO3]2 in fully polymerized sodium aluminosilicate melts and glasses. *Geochimica Et Cosmochimica Acta*, **1995**, 59, 683-698	5.5	38
113	Quantum mechanical modeling of the structures, energetics and spectral properties of I and I cellulose. *Cellulose*, **2013**, 20, 9-23	5.5	36
112	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
111	Structural factors affecting 13C NMR chemical shifts of cellulose: a computational study. *Cellulose*, **2018**, 25, 23-36	5.5	35
110	Interactions of biopolymers with silica surfaces: Force measurements and electronic structure calculation studies. *Geochimica Et Cosmochimica Acta*, **2006**, 70, 3803-3819	5.5	34
109	In situ structural characterization of ferric iron dimers in aqueous solutions: identification of oxo species. *Inorganic Chemistry*, **2013**, 52, 6788-97	5.1	33
108	Solid-state NMR and computational chemistry study of mononucleotides adsorbed to alumina. *Langmuir*, **2006**, 22, 9281-6	4	33
107	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
106	Faster proton transfer dynamics of water on SnO2 compared to TiO2. *Journal of Chemical Physics*, **2011**, 134, 044706	3.9	32
105	Molecular orbital modeling of aqueous organosilicon complexes: implications for silica biomineralization. *Geochimica Et Cosmochimica Acta*, **2003**, 67, 4113-4121	5.5	32
104	Effect of Ions on H-Bond Structure and Dynamics at the Quartz(101)-Water Interface. *Langmuir*, **2016**, 32, 11353-11365	4	31

103	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
102	Molecular orbital calculations for modeling acetate-aluminosilicate adsorption and dissolution reactions. *Geochimica Et Cosmochimica Acta*, **1997**, 61, 1031-1046	5.5	31
101	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
100	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
99	Molecular models of birnessite and related hydrated layered minerals. *American Mineralogist*, **2012**, 97, 1505-1514	2.9	29
98	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
97	Identification and characterization of a cellulose binding heptapeptide revealed by phage display. *Biomacromolecules*, **2013**, 14, 1795-805	6.9	27
96	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
95	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
94	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	5.5	26
93	Chemical diffusion in melts on the CaMgSi2O6-CaAl2Si2O8 join under high pressures. *Geochimica Et Cosmochimica Acta*, **1990**, 54, 2709-2715	5.5	26
92	Binding Geometries of Silicate Species on Ferrihydrite Surfaces. *ACS Earth and Space Chemistry*, **2018**, 2, 125-134	3.2	25
91	Quantum mechanical calculations on cellulosewater interactions: structures, energetics, vibrational frequencies and NMR chemical shifts for surfaces of Iand Icellulose. *Cellulose*, **2014**, 21, 909-926	5.5	25
90	Comparison of cation adsorption by isostructural rutile and cassiterite. *Langmuir*, **2011**, 27, 4585-93	4	25
89	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
88	Calculated trends of oh infrared stretching vibrations with composition and structure in aluminosilicate molecules. *Physics and Chemistry of Minerals*, **1993**, 20, 425	1.6	23
87	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
86	Reply to the comment by S.C. Kohn, M.E. Smith, and R. Dupree on A model for H2O solubility mechanisms in albite melts from infrared spectroscopy and molecular orbital calculations *Geochimica Et Cosmochimica Acta*, **1994**, 58, 1381-1384	5.5	22

85	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
84	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
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82	Plagioclase dissolution during CO2(g) sequestration: effects of sulfate. *Environmental Science & Technology*, **2015**, 49, 1946-54	10.3	19
81	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
80	Influence of glycosidic linkage neighbors on disaccharide conformation in vacuum. *Journal of Physical Chemistry B*, **2007**, 111, 13775-85	3.4	19
79	Deprotonation energies of a model fulvic acid. I. Carboxylic acid groups. *Geochimica Et Cosmochimica Acta*, **2006**, 70, 44-55	5.5	18
78	Comparison of As(III) and As(V) Complexation onto Al- and Fe-Hydroxides. *ACS Symposium Series*, **2005**, 104-117	0.4	18
77	Sustainable development of a surface-functionalized mesoporous aluminosilicate with ultra-high ion exchange efficiency. *Inorganic Chemistry Frontiers*, **2016**, 3, 502-513	6.8	17
76	Adsorption of carbon dioxide on Al/Fe oxyhydroxide. *Journal of Colloid and Interface Science*, **2013**, 400, 1-10	9.3	17
75	Adsorption of nitrate on kaolinite surfaces: a theoretical study. *Journal of Physical Chemistry B*, **2012**, 116, 11266-73	3.4	17
74	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
73	Hydrogen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. *Geochimica Et Cosmochimica Acta*, **2003**, 67, 1259-1276	5.5	17
72	Characterisation of gallium(III)-acetate complexes in aqueous solution: A potentiometric, EXAFS, IR and molecular orbital modelling study. *Dalton Transactions RSC*, **2002**, 2559-2564		17
71	Arabinose substitution effect on xylan rigidity and self-aggregation. *Cellulose*, **2019**, 26, 2267-2278	5.5	17
70	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
69	Interactions between aromatic hydrocarbons and functionalized C60 fullerenes: insights from experimental data and molecular modelling. *Environmental Science: Nano*, **2017**, 4, 1045-1053	7.1	15
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67	Description of Mg2+ Release from Forsterite Using Ab Initio Methods *Journal of Physical Chemistry C*, **2010**, 114, 5417-5428	3.8	15
66	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
65	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
64	Initiation, Elongation, and Termination of Bacterial Cellulose Synthesis. *ACS Omega*, **2018**, 3, 2690-2698	3.9	13
63	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
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59	Molecular models of benzene and selected polycyclic aromatic hydrocarbons in the aqueous and adsorbed states. *Environmental Toxicology and Chemistry*, **1999**, 18, 1656-1662	3.8	12
58	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
57	Competitive Adsorption of Acetic Acid and Water on Kaolinite. *Journal of Physical Chemistry A*, **2016** , 120, 8339-8346	2.8	11
56	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
55	Oxygen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. *Geochimica Et Cosmochimica Acta*, **2004**, 68, 949-958	5.5	11
54	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
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52	Interpretation of Vibrational Spectra Using Molecular Orbital Theory Calculations. *Reviews in Mineralogy and Geochemistry*, **2001**, 42, 459-483	7.1	11
51	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
50	Molecular modeling of Al3+ and benzene interactions with Suwannee fulvic acid. *Geochimica Et Cosmochimica Acta*, **2007**, 71, 3859-3871	5.5	10

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	Simultaneous Adsorption and Incorporation of Sr2+ at the Barite (001)Water Interface. *Journal of Physical Chemistry C*, **2019**, 123, 1194-1207	3.8	10
47	Quantum mechanical calculations on FeOH nanoparticles. *Geoderma*, **2012**, 189-190, 236-242	6.7	9
46	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
45	NMR spectroscopy of citrate in solids: cross-polarization kinetics in weakly coupled systems. *Magnetic Resonance in Chemistry*, **2008**, 46, 408-17	2.1	9
44	Simulations of Cellulose Synthesis Initiation and Termination in Bacteria. *Journal of Physical Chemistry B*, **2019**, 123, 3699-3705	3.4	8
43	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
42	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
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40	Quantum mechanical investigations of heme structure and vibrational spectra: effects of conformation, oxidation state, and electric field. *Langmuir*, **2009**, 25, 548-54	4	8
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38	Stereochemistry, elution order and molecular modeling of four diaergostanes in petroleum. *Organic Geochemistry*, **2014**, 76, 1-8	3.1	7
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