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	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
2	Ion Adsorption at the Rutileâ"Water Interface:Â Linking Molecular and Macroscopic Properties. Langmuir, 2004, 20, 4954-4969.	3.5	298
3	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
4	Development of a Reactive Force Field for Ironâ"Oxyhydroxide Systems. Journal of Physical Chemistry A, 2010, 114, 6298-6307.	2.5	199
5	Derivation of Force Field Parameters for TiO2â"H2O Systems from ab Initio Calculations. Journal of Physical Chemistry B, 2003, 107, 11072-11081.	2.6	196
6	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
7	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
8	Dissolution of nepheline, jadeite and albite glasses: toward better models for aluminosilicate dissolution. Geochimica Et Cosmochimica Acta, 2001, 65, 3683-3702.	3.9	180
9	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
10	ATR-FTIR spectroscopic characterization of coexisting carbonate surface complexes on hematite. Geochimica Et Cosmochimica Acta, 2005, 69, 1527-1542.	3.9	166
11	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
12	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
13	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
14	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
15	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
16	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
17	The Mechanism Responsible for Extraordinary Cs Ion Selectivity in Crystalline Silicotitanate. Journal of the American Chemical Society, 2008, 130, 11689-11694.	13.7	132
18	Probing cellulose structures with vibrational spectroscopy. Cellulose, 2019, 26, 35-79.	4.9	132

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19	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
20	Adhesion of Bacterial Exopolymers to Î±-FeOOH:Â Inner-Sphere Complexation of Phosphodiester Groups. Langmuir, 2004, 20, 11108-11114.	3.5	122
21	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
22	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
23	Bonding Mechanisms of Salicylic Acid Adsorbed onto Illite Clay:Â An ATRâ€“FTIR and Molecular Orbital Study. Environmental Science & Technology, 1997, 31, 1151-1156.	10.0	101
24	Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems. Langmuir, 2013, 29, 7838-7846.	3.5	96
25	X-ray Absorption Spectroscopic Quantification and Speciation Modeling of Sulfate Adsorption on Ferrihydrite Surfaces. Environmental Science & Technology, 2016, 50, 8067-8076.	10.0	96
26	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
27	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
28	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
29	Sum-Frequency-Generation Vibration Spectroscopy and Density Functional Theory Calculations with Dispersion Corrections (DFT-D2) for Cellulose Iβ and Iβ². Journal of Physical Chemistry B, 2013, 117, 6681-6692.	2.6	90
30	Models of natural organic matter and interactions with organic contaminants. Organic Geochemistry, 1999, 30, 911-927.	1.8	88
31	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
32	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
33	The Shape of Native Plant Cellulose Microfibrils. Scientific Reports, 2018, 8, 13983.	3.3	86
34	Ab Initio Calculation of Aqueous Aluminum and Aluminumâ€“Carboxylate Complex Energetics and 27Al NMR Chemical Shifts. Journal of Physical Chemistry A, 1999, 103, 903-915.	2.5	82
35	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
36	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

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37	Density Functional Theory Study of Ferrihydrite and Related Fe-Oxyhydroxides. Chemistry of Materials, 2009, 21, 5727-5742.	6.7	81
38	Ferrihydrite reactivity toward carbon dioxide. Journal of Colloid and Interface Science, 2009, 337, 492-500.	9.4	79
39	Cellulose Microfibril Twist, Mechanics, and Implication for Cellulose Biosynthesis. Journal of Physical Chemistry A, 2013, 117, 2580-2589.	2.5	79
40	Hydrogen Bonds and Vibrations of Water on (110) Rutile. Journal of Physical Chemistry C, 2009, 113, 13732-13740.	3.1	74
41	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
42	Theoretical and 27Al CPMAS NMR investigation of aluminum coordination changes during aluminosilicate dissolution. Geochimica Et Cosmochimica Acta, 2005, 69, 2205-2220.	3.9	72
43	Periodic density functional theory calculations of bulk and the (010) surface of goethite. Geochemical Transactions, 2008, 9, 4.	0.7	72
44	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
45	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
46	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
47	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
48	Molecular orbital calculations on aluminosilicate tricluster molecules: Implications for the structure of aluminosilicate glasses. American Mineralogist, 2002, 87, 668-678.	1.9	66
49	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
50	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
51	Effect of Dehydration on Sulfate Coordination and Speciation at the Feâ^'(Hydr)oxideâ^'Water Interface:Â A Molecular Orbital/Density Functional Theory and Fourier Transform Infrared Spectroscopic Investigation. Langmuir, 2005, 21, 11071-11078.	3.5	64
52	Quantum mechanical calculation of aqueuous uranium complexes: carbonate, phosphate, organic and biomolecular species. Chemistry Central Journal, 2009, 3, 10.	2.6	64
53	Surface Speciation of Phosphate on Boehmite (Î³-AlOOH) Determined from NMR Spectroscopy. Langmuir, 2010, 26, 4753-4761.	3.5	63
54	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

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55	Origin of Nanoscale Phase Stability Reversals in Titanium Oxide Polymorphs. Journal of Physical Chemistry C, 2009, 113, 4240-4245.	3.1	62
56	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
57	Four-membered rings in silica and aluminosilicate glasses. American Mineralogist, 1996, 81, 265-272.	1.9	58
58	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
59	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
60	Molecular dynamics simulations of the interactions between TiO₂ nanoparticles and water with Na⁺ and Cl^{â^'}, methanol, and formic acid using a reactive force field. Journal of Materials Research, 2013, 28, 513-520.	2.6	58
61	Arsenic Adsorption onto Minerals: Connecting Experimental Observations with Density Functional Theory Calculations. Minerals (Basel, Switzerland), 2014, 4, 208-240.	2.0	58
62	Molecular cluster models of aluminum oxide and aluminum hydroxide surfaces. American Mineralogist, 1998, 83, 1054-1066.	1.9	54
63	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
64	Theoretical reaction pathways for the formation of [Si(OH)5]1â^' and the deprotonation of orthosilicic acid in basic solution. Geochimica Et Cosmochimica Acta, 1993, 57, 3847-3853.	3.9	53
65	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
66	Photodissolution of Ferrihydrite in the Presence of Oxalic Acid: An In Situ ATR-FTIR/DFT Study. Langmuir, 2010, 26, 16246-16253.	3.5	53
67	High Temperature Microelectrophoresis Studies of the Rutile/Aqueous Solution Interface. Langmuir, 2003, 19, 3797-3804.	3.5	52
68	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
69	A New Hypothesis for the Dissolution Mechanism of Silicates. Journal of Physical Chemistry C, 2012, 116, 17479-17491.	3.1	52
70	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
71	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
72	Molecular orbital models of aqueous aluminum-acetate complexes. Geochimica Et Cosmochimica Acta, 1996, 60, 4897-4911.	3.9	48

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73	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
74	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
75	Solid-State NMR and Computational Chemistry Study of Mononucleotides Adsorbed to Alumina. Langmuir, 2006, 22, 9281-9286.	3.5	46
76	Molecular Simulations of Benzene and PAH Interactions with Soot. Environmental Science & Technology, 2006, 40, 2298-2303.	10.0	46
77	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
78	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	3.2	46
79	Structural factors affecting 13C NMR chemical shifts of cellulose: a computational study. Cellulose, 2018, 25, 23-36.	4.9	45
80	Mechanistic Aspects of Pyrite Oxidation in an Oxidizing Gaseous Environment:Â An in Situ HATRâ^'IR Isotope Study. Environmental Science & Technology, 2005, 39, 7576-7584.	10.0	43
81	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
82	Structural roles of CO2 and [CO3]2â^' in fully polymerized sodium aluminosilicate melts and glasses. Geochimica Et Cosmochimica Acta, 1995, 59, 683-698.	3.9	41
83	Gas-Phase Acidities of Tetrahedral Oxyacids from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2000, 104, 4051-4057.	2.5	41
84	Effect of Ions on H-Bond Structure and Dynamics at the Quartz(101)â€“Water Interface. Langmuir, 2016, 32, 11353-11365.	3.5	41
85	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
86	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
87	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
88	Quantum mechanical modeling of the structures, energetics and spectral properties of IÎ± and IÎ²2 cellulose. Cellulose, 2013, 20, 9-23.	4.9	39
89	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
90	Molecular orbital modeling of aqueous organosilicon complexes: implications for silica biomineralization. Geochimica Et Cosmochimica Acta, 2003, 67, 4113-4121.	3.9	37

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91	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
92	Molecular models of birnessite and related hydrated layered minerals. American Mineralogist, 2012, 97, 1505-1514.	1.9	36
93	Interactions of biopolymers with silica surfaces: Force measurements and electronic structure calculation studies. Geochimica Et Cosmochimica Acta, 2006, 70, 3803-3819.	3.9	35
94	Identification and Characterization of a Cellulose Binding Heptapeptide Revealed by Phage Display. Biomacromolecules, 2013, 14, 1795-1805.	5.4	35
95	Molecular orbital calculations for modeling acetate-aluminosilicate adsorption and dissolution reactions. Geochimica Et Cosmochimica Acta, 1997, 61, 1031-1046.	3.9	34
96	Faster proton transfer dynamics of water on SnO2 compared to TiO2. Journal of Chemical Physics, 2011, 134, 044706.	3.0	34
97	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
98	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
99	Arabinose substitution effect on xylan rigidity and self-aggregation. Cellulose, 2019, 26, 2267-2278.	4.9	31
100	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
101	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
102	Comparison of Cation Adsorption by Isostructural Rutile and Cassiterite. Langmuir, 2011, 27, 4585-4593.	3.5	29
103	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
104	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
105	Chemical diffusion in melts on the CaMgSi2O6-CaAl2Si2O8 join under high pressures. Geochimica Et Cosmochimica Acta, 1990, 54, 2709-2715.	3.9	27
106	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
107	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
108	Quantum mechanical calculations on celluloseâ€“water interactions: structures, energetics, vibrational frequencies and NMR chemical shifts for surfaces of Iİ± and Iİ² cellulose. Cellulose, 2014, 21, 909-926.	4.9	27

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109	Binding Geometries of Silicate Species on Ferrihydrite Surfaces. ACS Earth and Space Chemistry, 2018, 2, 125-134.	2.7	27
110	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
111	Density functional theory modeling of chromate adsorption onto ferrihydrite nanoparticles. Geochemical Transactions, 2018, 19, 8.	0.7	26
112	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
113	Plagioclase Dissolution during CO₂â€“SO₂ Cosequestration: Effects of Sulfate. Environmental Science & Technology, 2015, 49, 1946-1954.	10.0	23
114	Sustainable development of a surface-functionalized mesoporous aluminosilicate with ultra-high ion exchange efficiency. Inorganic Chemistry Frontiers, 2016, 3, 502-513.	6.0	23
115	Initiation, Elongation, and Termination of Bacterial Cellulose Synthesis. ACS Omega, 2018, 3, 2690-2698.	3.5	23
116	Adsorption of carbon dioxide on Al/Fe oxyhydroxide. Journal of Colloid and Interface Science, 2013, 400, 1-10.	9.4	22
117	Comparison of As(III) and As(V) Complexation onto Al- and Fe-Hydroxides. ACS Symposium Series, 2005, , 104-117.	0.5	21
118	Deprotonation energies of a model fulvic acid. I. Carboxylic acid groups. Geochimica Et Cosmochimica Acta, 2006, 70, 44-55.	3.9	21
119	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
120	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
121	Hydrogen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. Geochimica Et Cosmochimica Acta, 2003, 67, 1259-1276.	3.9	20
122	Description of Mg²⁺ Release from Forsterite Using Ab Initio Methods. Journal of Physical Chemistry C, 2010, 114, 5417-5428.	3.1	20
123	Adsorption of Nitrate on Kaolinite Surfaces: A Theoretical Study. Journal of Physical Chemistry B, 2012, 116, 11266-11273.	2.6	20
124	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
125	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
126	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

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127	Influence of Glycosidic Linkage Neighbors on Disaccharide Conformation in Vacuum. Journal of Physical Chemistry B, 2007, 111, 13775-13785.	2.6	19
128	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
129	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
130	Quantum Mechanical Modeling of the Vibrational Spectra of Minerals with a Focus on Clays. Minerals (Basel, Switzerland), 2019, 9, 141.	2.0	18
131	Interpretation of Vibrational Spectra Using Molecular Orbital Theory Calculations. Reviews in Mineralogy and Geochemistry, 2001, 42, 459-483.	4.8	17
132	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
133	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
134	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
135	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
136	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
137	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
138	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
139	Competitive Adsorption of Acetic Acid and Water on Kaolinite. Journal of Physical Chemistry A, 2016, 120, 8339-8346.	2.5	14
140	Oxygen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. Geochimica Et Cosmochimica Acta, 2004, 68, 949-958.	3.9	13
141	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
142	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
143	In silico structure prediction of full-length cotton cellulose synthase protein (GhCESA1) and its hierarchical complexes. Cellulose, 2020, 27, 5597-5616.	4.9	13
144	Molecular Orbital Modeling and Transition State Theory in Geochemistry. Reviews in Mineralogy and Geochemistry, 2001, 42, 485-531.	4.8	12

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145	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
146	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
147	Stereochemistry, elution order and molecular modeling of four diaergostanes in petroleum. Organic Geochemistry, 2014, 76, 1-8.	1.8	12
148	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
149	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
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