Daniel Tunega

List of Publications by Year
in descending order

126	3,774	94269 37	155451 55
papers	citations	h-index	g-index

128	128	128	3614
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Wettability of kaolinite (001) surfaces â€" Molecular dynamic study. Geoderma, 2011, 169, 47-54.	2.3	176
2	Solvent Effects on Hydrogen BondsA Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 1862-1871.	1.1	167
3	Ab Initio Molecular Dynamics Study of a Monomolecular Water Layer on Octahedral and Tetrahedral Kaolinite Surfaces. Journal of Physical Chemistry B, 2004, 108, 5930-5936.	1.2	146
4	Assessment of ten DFT methods in predicting structures of sheet silicates: Importance of dispersion corrections. Journal of Chemical Physics, 2012, 137, 114105.	1.2	117
5	Upper Limit of the Oâ˜HÂ·Â·Â·O Hydrogen Bond. Ab Initio Study of the Kaolinite Structure. Journal of Physical Chemistry B, 2001, 105, 10812-10817.	1.2	109
6	Theoretical Study of Adsorption Sites on the (001) Surfaces of 1:1 Clay Minerals. Langmuir, 2002, 18, 139-147.	1.6	106
7	Ab Initio Molecular Dynamics Study of Adsorption Sites on the (001) Surfaces of 1:1 Dioctahedral Clay Minerals. Journal of Physical Chemistry B, 2002, 106, 11515-11525.	1.2	105
8	Orientation of OH groups in kaolinite and dickite: Ab initio molecular dynamics study. American Mineralogist, 2001, 86, 1057-1065.	0.9	98
9	The interplay of skeletal deformations and ultrafast excited-state intramolecular proton transfer: Experimental and theoretical investigation of 10-hydroxybenzo[h]quinoline. Chemical Physics, 2008, 347, 446-461.	0.9	91
10	Free radicals generated during oxidation of green tea polyphenols: Electron paramagnetic resonance spectroscopy combined with density functional theory calculations. Free Radical Biology and Medicine, 2009, 46, 1076-1088.	1.3	74
11	Density Functional Theory (DFT) Study of the Hydration Steps of Na⁺/Mg²⁺/Ca²⁺/Sr²⁺/Ba²⁺-Exchanged Montmorillonites. Clays and Clay Minerals, 2010, 58, 174-187.	0.6	72
12	Glass formation and structure in the system Cu2Oî—¸P2O5î—¸MoO3. Journal of Non-Crystalline Solids, 1995, 185, 151-158.	1.5	71
13	Molecular Dynamics Simulations of the Standard Leonardite Humic Acid: Microscopic Analysis of the Structure and Dynamics. Environmental Science & Technology, 2017, 51, 5414-5424.	4.6	71
14	The performance of the explicitly correlated coupled cluster method. I. The fourâ€electron systems Be, Liâ˜, and LiH. Journal of Chemical Physics, 1995, 103, 309-320.	1.2	67
15	Structural and spectroscopic characterization of ettringite mineral â€"combined DFT and experimental study. Journal of Molecular Structure, 2015, 1100, 215-224.	1.8	59
16	Theoretical study of interactions of dickite and kaolinite with small organic molecules. Computational and Theoretical Chemistry, 2002, 581, 37-49.	1.5	55
17	Molecular Dynamics Simulations of Water Molecule-Bridges in Polar Domains of Humic Acids. Environmental Science & Technology, 2011, 45, 8411-8419.	4.6	54
18	Acidâ€"base properties of a goethite surface model: A theoretical view. Geochimica Et Cosmochimica Acta, 2008, 72, 3587-3602.	1.6	50

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19	Fluorination of an Alumina Surface: Modeling Aluminumâ€“Fluorine Reaction Mechanisms. ACS Applied Materials & Interfaces, 2017, 9, 24290-24297.	4.0	49
20	Stabilizing Capacity of Water Bridges in Nanopore Segments of Humic Substances: A Theoretical Investigation. Journal of Physical Chemistry C, 2009, 113, 16468-16475.	1.5	47
21	The functionality of cation bridges for binding polar groups in soil aggregates. International Journal of Quantum Chemistry, 2011, 111, 1531-1542.	1.0	46
22	Influence of Synthesis Conditions on the Formation of a Kaolinitemethanol Complex and Simulation of its Vibrational Spectra. Clays and Clay Minerals, 2012, 60, 227-239.	0.6	46
23	Theoretical Study of Properties of Goethite (Î±-FeOOH) at Ambient and High-Pressure Conditions. Journal of Physical Chemistry C, 2012, 116, 6703-6713.	1.5	46
24	Response of sorption processes of MCPA to the amount and origin of organic matter in a long-term field experiment. European Journal of Soil Science, 2001, 52, 279-286.	1.8	45
25	Ab initio density functional theory applied to the structure and proton dynamics of clays. Chemical Physics Letters, 2001, 333, 479-484.	1.2	45
26	Static electric properties of LiH: explicitly correlated coupled cluster calculations. Theoretical Chemistry Accounts, 1998, 100, 78-84.	0.5	44
27	Interaction of Acetate Anion with Hydrated Al3+Cation:Â A Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 6824-6833.	1.1	44
28	Theoretical and experimental study of montmorillonite intercalated with tetramethylammonium cation. Vibrational Spectroscopy, 2013, 66, 123-131.	1.2	42
29	A density-functional investigation of aluminium(III)â€“citrate complexes. Physical Chemistry Chemical Physics, 2001, 3, 1979-1985.	1.3	41
30	Kaolinite:Dimethylsulfoxide IntercalateA Theoretical Study. Journal of Physical Chemistry C, 2007, 111, 11259-11266.	1.5	41
31	Ab Initio Study of Structure and Interconversion of Native Cellulose Phases. Journal of Physical Chemistry A, 2011, 115, 10097-10105.	1.1	41
32	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.	1.4	41
33	Interaction of the 2,4-dichlorophenoxyacetic acid herbicide with soil organic matter moieties: a theoretical study. European Journal of Soil Science, 2007, 58, 889-899.	1.8	40
34	Adsorption of organic substances on broken clay surfaces: A quantum chemical study. Journal of Computational Chemistry, 2003, 24, 1853-1863.	1.5	39
35	Quantum Chemical Adsorption Studies on the (110) Surface of the Mineral Goethite. Journal of Physical Chemistry C, 2007, 111, 877-885.	1.5	39
36	Adsorption of the Herbicide 4-Chloro-2-methylphenoxyacetic Acid (MCPA) by Goethite. Environmental Science & Technology, 2014, 48, 11803-11810.	4.6	38

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37	The thermodynamic stability of hydrogen bonded and cation bridged complexes of humic acid modelsâ€"A theoretical study. Chemical Physics, 2008, 349, 69-76.	0.9	37
38	Model study on sorption of polycyclic aromatic hydrocarbons to goethite. Journal of Colloid and Interface Science, 2009, 330, 244-249.	5.0	37
39	External surface structure of organoclays analyzed by transmission electron microscopy and X-ray photoelectron spectroscopy in combination with molecular dynamics simulations. Journal of Colloid and Interface Science, 2016, 478, 188-200.	5.0	37
40	Modeling Catalytic Effects of Clay Mineral Surfaces on Peptide Bond Formation. Journal of Physical Chemistry B, 2004, 108, 10120-10130.	1.2	36
41	Basis set limit value for the static dipole polarizability of beryllium. Chemical Physics Letters, 1997, 269, 435-440.	1.2	33
42	The combined inelastic neutron scattering and solid state DFT study of hydrogen atoms dynamics in a highly ordered kaolinite. Physics and Chemistry of Minerals, 2010, 37, 571-579.	0.3	33
43	Understanding of bonding and mechanical characteristics of cementitious mineral tobermorite from first principles. Journal of Computational Chemistry, 2011, 32, 306-314.	1.5	33
44	Vienna Soil-Organic-Matter Modelerâ€"Generating condensed-phase models of humic substances. Journal of Molecular Graphics and Modelling, 2015, 62, 253-261.	1.3	33
45	Interaction between Cellobiose Dehydrogenase and Lytic Polysaccharide Monooxygenase. Biochemistry, 2019, 58, 1226-1235.	1.2	32
46	Surface structure of organoclays as examined by X-ray photoelectron spectroscopy and molecular dynamics simulations. Clay Minerals, 2015, 50, 353-367.	0.2	31
47	A density functional theoretical study on solvated Al3+â€"oxalate complexes: structures and thermodynamic properties. Physical Chemistry Chemical Physics, 2000, 2, 2845-2850.	1.3	30
48	Iron Nitride Nanoparticles for Enhanced Reductive Dechlorination of Trichloroethylene. Environmental Science & Technology, 2022, 56, 4425-4436.	4.6	30
49	Formation of 2,4?D complexes on montmorillonites ? an ab initio molecular dynamics study. European Journal of Soil Science, 2007, 58, 680-691.	1.8	29
50	Mechanical properties of ettringite and thaumasiteâ€"DFT and experimental study. Cement and Concrete Research, 2015, 77, 9-15.	4.6	29
51	Adsorption of phenanthrene on Na-montmorillonite: A model study. Geoderma, 2011, 169, 41-46.	2.3	27
52	SORPTION OF PHENOXYACETIC ACID HERBICIDES ON THE KAOLINITE MINERAL SURFACE â€" AN AB INITIO MOLECULAR DYNAMICS SIMULATION. Soil Science, 2004, 169, 44-54.	0.9	26
53	Study of solvent effect on the stability of water bridge-linked carboxyl groups in humic acid models. Geoderma, 2011, 169, 20-26.	2.3	26
54	<I>Ab initio</I> calculations of relative stabilities of different structural arrangements in dioctahedral phyllosilicates. Clays and Clay Minerals, 2007, 55, 220-232.	0.6	24

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55	Thermodynamic stability of hydrogenâ€bonded systems in polar and nonpolar environments. Journal of Computational Chemistry, 2010, 31, 2046-2055.	1.5	24
56	Restructuring of a Peat in Interaction with Multivalent Cations: Effect of Cation Type and Aging Time. PLoS ONE, 2013, 8, e65359.	1.1	24
57	Theoretical study of cation substitution in trioctahedral sheet of phyllosilicates. An effect on inner OH group. Computational and Theoretical Chemistry, 2003, 620, 1-8.	1.5	23
58	Sorption of naphthalene derivatives to soils from a long-term field experiment. Chemosphere, 2005, 59, 639-647.	4.2	23
59	A model study of dickite intercalated with formamide and N-methylformamide. Physics and Chemistry of Minerals, 2008, 35, 299-309.	0.3	22
60	Radical sites in humic acids: A theoretical study on protocatechuic and gallic acids. Computational and Theoretical Chemistry, 2014, 1032, 42-49.	1.1	22
61	Experimental and molecular dynamics study on anion diffusion in organically modified bentonite. Applied Clay Science, 2016, 120, 91-100.	2.6	22
62	Mechanical and Bonding Behaviors Behind the Bending Mechanism of Kaolinite Clay Layers. Journal of Physical Chemistry C, 2020, 124, 7432-7440.	1.5	21
63	Experimental and computational study of thaumasite structure. Cement and Concrete Research, 2014, 59, 66-72.	4.6	20
64	Polarization Effects in Simulations of Kaoliniteâ€“Water Interfaces. Langmuir, 2019, 35, 15086-15099.	1.6	19
65	Prediction of mechanical properties of grafted kaolinite â€“ A DFT study. Applied Clay Science, 2020, 193, 105692.	2.6	19
66	Soil organic matter stabilization at molecular scale: The role of metal cations and hydrogen bonds. Geoderma, 2021, 401, 115237.	2.3	19
67	Structural and Spectroscopic Characterization of Montmorillonite Intercalated with N-Butylammonium Cations (N = 1-4) â€” Modeling and Experimental Study. Clays and Clay Minerals, 2016, 64, 401-412.	0.6	19
68	Adsorption of H2O, NH3 and C6H6 on alkali metal cations in internal surface of mordenite and in external surface of smectite: a DFT study. Physics and Chemistry of Minerals, 2009, 36, 281-290.	0.3	18
69	Theoretical study of structural, mechanical and spectroscopic properties of boehmite (Î³-AlOOH). Journal of Physics Condensed Matter, 2011, 23, 404201.	0.7	18
70	The stability of the acetic acid dimer in microhydrated environments and in aqueous solution. Physical Chemistry Chemical Physics, 2012, 14, 4162.	1.3	18
71	Comparison of Cluster, Slab, and Analytic Potential Models for the Dimethyl Methylphosphonate (DMMP)/TiO₂(110) Intermolecular Interaction. Journal of Physical Chemistry C, 2013, 117, 17613-17622.	1.5	18
72	Free radical generation in rosmarinic acid investigated by electron paramagnetic resonance spectroscopy. Free Radical Research, 2009, 43, 47-57.	1.5	17

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73	Structural properties of montmorillonite intercalated with tetraalkylammonium cationsâ€"Computational and experimental study. Vibrational Spectroscopy, 2014, 74, 120-126.	1.2	17
74	Effect of Polar Environments on the Aluminum Oxide Shell Surrounding Aluminum Particles: Simulations of Surface Hydroxyl Bonding and Charge. ACS Applied Materials & Interfaces, 2016, 8, 13926-13933.	4.0	17
75	Molecular modelling of sorption processes of a range of diverse small organic molecules in Leonardite humic acid. European Journal of Soil Science, 2020, 71, 831-844.	1.8	16
76	Effect of the Si/Al ordering on structural parameters and the energetic stabilization of vermiculites ? a theoretical study. Physics and Chemistry of Minerals, 2003, 30, 517-522.	0.3	15
77	The Combined Inelastic Neutron Scattering (INS) and Solid-State DFT Study of Hydrogen-Atoms Dynamics in Kaolinite-dimethylsulfoxide Intercalate. Clays and Clay Minerals, 2010, 58, 52-61.	0.6	15
78	Bonds, bands and elasticity of smithsonite rock. Solid State Communications, 2013, 166, 76-82.	0.9	15
79	A contribution of molecular modeling to supramolecular structures in soil organic matter[#]. Journal of Plant Nutrition and Soil Science, 2022, 185, 44-59.	1.1	14
80	Structure and physical properties of stabilized HfO2-R2O3 (R = Sc, Yb, Y, Tb, Gd, Er). Materials Chemistry and Physics, 1993, 34, 175-180.	2.0	12
81	Proton transfer processes in polar regions of humic substances initiated by aqueous aluminum cation bridges: A computational study. Geoderma, 2014, 213, 115-123.	2.3	12
82	Cationâ€"Ï€ interactions in competition with cation microhydration: a theoretical study of alkali metal cationâ€"pyrene complexes. Journal of Molecular Modeling, 2017, 23, 131.	0.8	12
83	Low-frequency vibrational modes in fluorite based superionic conductors - Raman study. Solid State Ionics, 1992, 58, 237-242.	1.3	11
84	Proton exchange reactions of C2â€"C4 alkanes sorbed in ZSM-5 zeolite. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	11
85	Adsorption process of polar and nonpolar compounds in a nanopore model of humic substances. European Journal of Soil Science, 2020, 71, 845-855.	1.8	11
86	Density functional theory study of the stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. Clay Minerals, 2019, 54, 41-48.	0.2	11
87	On glyphosateâ€"kaolinite surface interactions. A molecular dynamic study. European Journal of Soil Science, 2021, 72, 1231-1242.	1.8	11
88	A Study of the Disorder in Heavily Doped Ba_{1â€"x}La_xF_{2+x} by Raman Scattering. Physica Status Solidi (B): Basic Research, 1990, 160, 375-380.	0.7	10
89	The influence of tungsten on the oxygen sublattice in yttria-stabilized zirconia (YSZ). Solid State Ionics, 1995, 76, 207-214.	1.3	10
90	Stability of Tetrabutylphosphonium Beidellite Organoclay. Journal of Physical Chemistry C, 2018, 122, 8380-8389.	1.5	10

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91	Inelastic neutron scattering and DFT study of 1,6-anhydro-Î²-d-glucopyranose (levoglucosan). Journal of Molecular Structure, 2008, 874, 108-120.	1.8	9
92	A theoretical study of adsorption on iron sulfides towards nanoparticle modeling. Physical Chemistry Chemical Physics, 2020, 22, 23258-23267.	1.3	9
93	Second-degree twinning and dynamic disorder in the crystal structure of deca-dodecasil 3R. Acta Crystallographica Section B: Structural Science, 2005, 61, 627-634.	1.8	8
94	Multiple adsorption of NO on cobalt-exchanged chabazite, mordenite, and ferrierite zeolites: A periodic density functional theory study. Journal of Chemical Physics, 2009, 131, 054101.	1.2	8
95	Effect of Hydration on Promoting Oxidative Reactions with Aluminum Oxide and Oxyhydroxide Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 15017-15026.	1.5	8
96	Stress-altered aluminum powder dust combustion. Journal of Applied Physics, 2020, 127, .	1.1	7
97	Regulating magnesium combustion using surface chemistry and heating rate. Combustion and Flame, 2021, 226, 419-429.	2.8	7
98	Adsorption of polycyclic aromatic hydrocarbons on FeOOH polymorphs: A theoretical study. Surface Science, 2021, 706, 121795.	0.8	7
99	Preparation, characterization and adsorption properties of tetraalkylphosphonium organobeidellites. Applied Clay Science, 2021, 204, 105989.	2.6	7
100	Stability of Atrazineâ€“Smectite Intercalates: Density Functional Theory and Experimental Study. Minerals (Basel, Switzerland), 2021, 11, 554.	0.8	7
101	Advances of molecular modeling of biogeochemical interfaces in soils. Geoderma, 2011, 169, 1-3.	2.3	6
102	The structure and energetics of cryolite melts. Theoretical Chemistry Accounts, 1998, 99, 378-383.	0.5	5
103	Ab initio 2-D periodic Hartree-Fock study of Fe-substituted lizardite 1 T - a simplified cronstedtite model. Physics and Chemistry of Minerals, 2000, 27, 741-746.	0.3	5
104	Ab Initio Molecular Dynamics Simulations on the Hydrated Structures of Na+â€“Nafion Models. Journal of Physical Chemistry C, 2017, 121, 11215-11225.	1.5	5
105	On the Adsorption Mechanism of Humic Substances on Kaolinite and Their Microscopic Structure. Minerals (Basel, Switzerland), 2021, 11, 1138.	0.8	5
106	Interaction of naphthalene derivatives with soil: an experimental and theoretical case study. European Journal of Soil Science, 2007, 58, 967-977.	1.8	4
107	Sorption of Selected Aromatic Substancesâ€”Application of Kinetic Concepts and Quantum Mechanical Modeling. Water, Air, and Soil Pollution, 2011, 215, 449-464.	1.1	4
108	Wettability of organically coated tridymite surface â€“ molecular dynamics study. Pure and Applied Chemistry, 2015, 87, 405-413.	0.9	4

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109	Synthesis and characterization of polymeric films with stress-altered aluminum particle fillers. Journal of Materials Science, 2020, 55, 14229-14242.	1.7	4
110	Geometry and molecular arrangement of phosphatidylcholine-montmorillonite bioclays via classical molecular dynamics simulation. Applied Clay Science, 2020, 198, 105815.	2.6	4
111	Molecular Models of Cation and Water Molecule Bridges in Humic Substances. , 2014, , 107-115.		4
112	Insights on the Structural and Dynamic Properties of Corundumâ€“Water Interfaces from First-Principle Molecular Dynamics. Journal of Physical Chemistry C, 2021, 125, 295-309.	1.5	4
113	Microhydration of Polymer Electrolyte Membranes: A Comparison of Hydrogen-Bonding Networks and Spectral Properties of Nafion and Bis[(perfluoroalkyl)sulfonyl] Imide. Journal of Physical Chemistry B, 2019, 123, 9899-9911.	1.2	3
114	Influence of water molecule bridges on sequestration of phenol in soil organic matter of sapric histosol. Environmental Chemistry, 2019, 16, 541.	0.7	3
115	Molecular modeling of MCPA herbicide adsorption by goethite (110) surface in dependence of pH. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	3
116	Inelastic neutron scattering and DFT study of 2-amino-3-hydroxymethyl-1,3-propane diol (TRIS). Chemical Physics, 2007, 340, 245-259.	0.9	2
117	Reaction mechanism for fluorination reactions with hydroxylated alumina sites: Pathways promoting aluminum combustion. Journal of Chemical Physics, 2021, 154, 104308.	1.2	2
118	Theoretical study of the electrostatic potential of an idealized semi-infinite crystal of talc and vibrational frequencies of an adsorbed proton. Physics and Chemistry of Minerals, 1994, 21, 213.	0.3	1
119	Editorial: Molecular modelling in soil research. European Journal of Soil Science, 2007, 58, 867-869.	1.8	1
120	Hydrogen Bonds And Solvent Effects In Soil Processes: A Theoretical View. Challenges and Advances in Computational Chemistry and Physics, 2008, , 321-347.	0.6	1
121	Hydrophobicity and Charge Distribution Effects in the Formation of Bioorganoclays. Minerals (Basel,) Tj ETQq1 1 0.784314 rgBT /Over	0.8	1
122	Disordering of oxygen sublattice in Cr-doped YSZ. Ferroelectrics, 1996, 176, 203-212.	0.3	0
123	Model Study of Partial Structural Decomposition of Thaumasite. Applied Mechanics and Materials, 2015, 749, 8-12.	0.2	0
124	Solvent effect on Al(III) hydrolysis constants from density functional theory. Molecular Physics, 2019, 117, 1507-1518.	0.8	0
125	Soil organic matter in molecular simulations. , 2022, , .		0
126	Adsorption and exchange reactions of iodine molecules at the alumina surface: modelling alumina-iodine reaction mechanisms. Physical Chemistry Chemical Physics, 2022, , .	1.3	0