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	Soil organic matter in molecular simulations. , 2022, , .		0
2	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
3	Adsorption and exchange reactions of iodine molecules at the alumina surface: modelling alumina-iodine reaction mechanisms. Physical Chemistry Chemical Physics, 2022, , .	1.3	0
4	Iron Nitride Nanoparticles for Enhanced Reductive Dechlorination of Trichloroethylene. Environmental Science & Technology, 2022, 56, 4425-4436.	4.6	30
5	On glyphosateâ€“kaolinite surface interactions. A molecular dynamic study. European Journal of Soil Science, 2021, 72, 1231-1242.	1.8	11
6	Reaction mechanism for fluorination reactions with hydroxylated alumina sites: Pathways promoting aluminum combustion. Journal of Chemical Physics, 2021, 154, 104308.	1.2	2
7	Regulating magnesium combustion using surface chemistry and heating rate. Combustion and Flame, 2021, 226, 419-429.	2.8	7
8	Adsorption of polycyclic aromatic hydrocarbons on FeOOH polymorphs: A theoretical study. Surface Science, 2021, 706, 121795.	0.8	7
9	Preparation, characterization and adsorption properties of tetraalkylphosphonium organobeidellites. Applied Clay Science, 2021, 204, 105989.	2.6	7
10	Stability of Atrazineâ€“Smectite Intercalates: Density Functional Theory and Experimental Study. Minerals (Basel, Switzerland), 2021, 11, 554.	0.8	7
11	Soil organic matter stabilization at molecular scale: The role of metal cations and hydrogen bonds. Geoderma, 2021, 401, 115237.	2.3	19
12	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
13	Hydrophobicity and Charge Distribution Effects in the Formation of Bioorganoclays. Minerals (Basel,) Tj ETQq1 1 0.784314 rgBT /Over	0.8	1
14	On the Adsorption Mechanism of Humic Substances on Kaolinite and Their Microscopic Structure. Minerals (Basel, Switzerland), 2021, 11, 1138.	0.8	5
15	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
16	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
17	Synthesis and characterization of polymeric films with stress-altered aluminum particle fillers. Journal of Materials Science, 2020, 55, 14229-14242.	1.7	4
18	Molecular modeling of MCPA herbicide adsorption by goethite (110) surface in dependence of pH. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	3

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19	A theoretical study of adsorption on iron sulfides towards nanoparticle modeling. Physical Chemistry Chemical Physics, 2020, 22, 23258-23267.	1.3	9
20	Geometry and molecular arrangement of phosphatidylcholine-montmorillonite bioclays via classical molecular dynamics simulation. Applied Clay Science, 2020, 198, 105815.	2.6	4
21	Stress-altered aluminum powder dust combustion. Journal of Applied Physics, 2020, 127, .	1.1	7
22	Prediction of mechanical properties of grafted kaolinite â€“ A DFT study. Applied Clay Science, 2020, 193, 105692.	2.6	19
23	Mechanical and Bonding Behaviors Behind the Bending Mechanism of Kaolinite Clay Layers. Journal of Physical Chemistry C, 2020, 124, 7432-7440.	1.5	21
24	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
25	Polarization Effects in Simulations of Kaoliniteâ€“Water Interfaces. Langmuir, 2019, 35, 15086-15099.	1.6	19
26	Solvent effect on Al(III) hydrolysis constants from density functional theory. Molecular Physics, 2019, 117, 1507-1518.	0.8	0
27	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
28	Interaction between Cellobiose Dehydrogenase and Lytic Polysaccharide Monooxygenase. Biochemistry, 2019, 58, 1226-1235.	1.2	32
29	Density functional theory study of the stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. Clay Minerals, 2019, 54, 41-48.	0.2	11
30	Influence of water molecule bridges on sequestration of phenol in soil organic matter of sapric histosol. Environmental Chemistry, 2019, 16, 541.	0.7	3
31	Stability of Tetrabutylphosphonium Beidellite Organoclay. Journal of Physical Chemistry C, 2018, 122, 8380-8389.	1.5	10
32	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
33	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
34	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
35	Fluorination of an Alumina Surface: Modeling Aluminumâ€“Fluorine Reaction Mechanisms. ACS Applied Materials & Interfaces, 2017, 9, 24290-24297.	4.0	49
36	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

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37	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
38	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
39	Experimental and molecular dynamics study on anion diffusion in organically modified bentonite. Applied Clay Science, 2016, 120, 91-100.	2.6	22
40	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
41	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
42	Model Study of Partial Structural Decomposition of Thaumasite. Applied Mechanics and Materials, 2015, 749, 8-12.	0.2	0
43	Surface structure of organoclays as examined by X-ray photoelectron spectroscopy and molecular dynamics simulations. Clay Minerals, 2015, 50, 353-367.	0.2	31
44	Structural and spectroscopic characterization of ettringite mineral â€"combined DFT and experimental study. Journal of Molecular Structure, 2015, 1100, 215-224.	1.8	59
45	Wettability of organically coated tridymite surface â€" molecular dynamics study. Pure and Applied Chemistry, 2015, 87, 405-413.	0.9	4
46	Mechanical properties of ettringite and thaumasiteâ€"DFT and experimental study. Cement and Concrete Research, 2015, 77, 9-15.	4.6	29
47	Experimental and computational study of thaumasite structure. Cement and Concrete Research, 2014, 59, 66-72.	4.6	20
48	Radical sites in humic acids: A theoretical study on protocatechuic and gallic acids. Computational and Theoretical Chemistry, 2014, 1032, 42-49.	1.1	22
49	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
50	Adsorption of the Herbicide 4-Chloro-2-methylphenoxyacetic Acid (MCPA) by Goethite. Environmental Science & Technology, 2014, 48, 11803-11810.	4.6	38
51	Structural properties of montmorillonite intercalated with tetraalkylammonium cationsâ€"Computational and experimental study. Vibrational Spectroscopy, 2014, 74, 120-126.	1.2	17
52	Molecular Models of Cation and Water Molecule Bridges in Humic Substances. , 2014, , 107-115.		4
53	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
54	Theoretical and experimental study of montmorillonite intercalated with tetramethylammonium cation. Vibrational Spectroscopy, 2013, 66, 123-131.	1.2	42

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55	Bonds, bands and elasticity of smithsonite rock. Solid State Communications, 2013, 166, 76-82.	0.9	15
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	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
58	The stability of the acetic acid dimer in microhydrated environments and in aqueous solution. Physical Chemistry Chemical Physics, 2012, 14, 4162.	1.3	18
59	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
60	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
61	Proton exchange reactions of C2â€“C4 alkanes sorbed in ZSM-5 zeolite. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	11
62	Theoretical study of structural, mechanical and spectroscopic properties of boehmite (Î³-AlOOH). Journal of Physics Condensed Matter, 2011, 23, 404201.	0.7	18
63	Molecular Dynamics Simulations of Water Molecule-Bridges in Polar Domains of Humic Acids. Environmental Science & Technology, 2011, 45, 8411-8419.	4.6	54
64	Ab Initio Study of Structure and Interconversion of Native Cellulose Phases. Journal of Physical Chemistry A, 2011, 115, 10097-10105.	1.1	41
65	Adsorption of phenanthrene on Na-montmorillonite: A model study. Geoderma, 2011, 169, 41-46.	2.3	27
66	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
67	Wettability of kaolinite (001) surfaces â€" Molecular dynamic study. Geoderma, 2011, 169, 47-54.	2.3	176
68	Advances of molecular modeling of biogeochemical interfaces in soils. Geoderma, 2011, 169, 1-3.	2.3	6
69	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
70	The functionality of cation bridges for binding polar groups in soil aggregates. International Journal of Quantum Chemistry, 2011, 111, 1531-1542.	1.0	46
71	Understanding of bonding and mechanical characteristics of cementitious mineral tobermorite from first principles. Journal of Computational Chemistry, 2011, 32, 306-314.	1.5	33
72	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

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73	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
74	Thermodynamic stability of hydrogenâ€bonded systems in polar and nonpolar environments. Journal of Computational Chemistry, 2010, 31, 2046-2055.	1.5	24
75	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
76	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
77	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
78	Model study on sorption of polycyclic aromatic hydrocarbons to goethite. Journal of Colloid and Interface Science, 2009, 330, 244-249.	5.0	37
79	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
80	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
81	Free radical generation in rosmarinic acid investigated by electron paramagnetic resonance spectroscopy. Free Radical Research, 2009, 43, 47-57.	1.5	17
82	A model study of dickite intercalated with formamide and N-methylformamide. Physics and Chemistry of Minerals, 2008, 35, 299-309.	0.3	22
83	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
84	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
85	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
86	Acidâ€"base properties of a goethite surface model: A theoretical view. Geochimica Et Cosmochimica Acta, 2008, 72, 3587-3602.	1.6	50
87	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
88	<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
89	Quantum Chemical Adsorption Studies on the (110) Surface of the Mineral Goethite. Journal of Physical Chemistry C, 2007, 111, 877-885.	1.5	39
90	Kaolinite:Dimethylsulfoxide IntercalateA Theoretical Study. Journal of Physical Chemistry C, 2007, 111, 11259-11266.	1.5	41

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91	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
92	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
93	Editorial: Molecular modelling in soil research. European Journal of Soil Science, 2007, 58, 867-869.	1.8	1
94	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
95	Interaction of naphthalene derivatives with soil: an experimental and theoretical case study. European Journal of Soil Science, 2007, 58, 967-977.	1.8	4
96	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
97	Sorption of naphthalene derivatives to soils from a long-term field experiment. Chemosphere, 2005, 59, 639-647.	4.2	23
98	Modeling Catalytic Effects of Clay Mineral Surfaces on Peptide Bond Formation. Journal of Physical Chemistry B, 2004, 108, 10120-10130.	1.2	36
99	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
100	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
101	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
102	Adsorption of organic substances on broken clay surfaces: A quantum chemical study. Journal of Computational Chemistry, 2003, 24, 1853-1863.	1.5	39
103	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
104	Solvent Effects on Hydrogen BondsA Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 1862-1871.	1.1	167
105	Theoretical Study of Adsorption Sites on the (001) Surfaces of 1:1 Clay Minerals. Langmuir, 2002, 18, 139-147.	1.6	106
106	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
107	Theoretical study of interactions of dickite and kaolinite with small organic molecules. Computational and Theoretical Chemistry, 2002, 581, 37-49.	1.5	55
108	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

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109	A density-functional investigation of aluminium(III)â€“citrate complexes. Physical Chemistry Chemical Physics, 2001, 3, 1979-1985.	1.3	41
110	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
111	Ab initio density functional theory applied to the structure and proton dynamics of clays. Chemical Physics Letters, 2001, 333, 479-484.	1.2	45
112	Orientation of OH groups in kaolinite and dickite: Ab initio molecular dynamics study. American Mineralogist, 2001, 86, 1057-1065.	0.9	98
113	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
114	Interaction of Acetate Anion with Hydrated Al3+Cation:Â A Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 6824-6833.	1.1	44
115	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
116	The structure and energetics of cryolite melts. Theoretical Chemistry Accounts, 1998, 99, 378-383.	0.5	5
117	Static electric properties of LiH: explicitly correlated coupled cluster calculations. Theoretical Chemistry Accounts, 1998, 100, 78-84.	0.5	44
118	Basis set limit value for the static dipole polarizability of beryllium. Chemical Physics Letters, 1997, 269, 435-440.	1.2	33
119	Disordering of oxygen sublattice in Cr-doped YSZ. Ferroelectrics, 1996, 176, 203-212.	0.3	0
120	The influence of tungsten on the oxygen sublattice in yttria-stabilized zirconia (YSZ). Solid State Ionics, 1995, 76, 207-214.	1.3	10
121	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
122	Glass formation and structure in the system Cu2Oî—¸P2O5î—¸MoO3. Journal of Non-Crystalline Solids, 1995, 185, 151-158.	1.5	71
123	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
124	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
125	Low-frequency vibrational modes in fluorite based superionic conductors - Raman study. Solid State Ionics, 1992, 58, 237-242.	1.3	11
126	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