Randall T Cygan

List of Publications by Year
in descending order

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97 papers	7,809 citations	53794 45 h-index	49909 87 g-index
100 all docs	100 docs citations	100 times ranked	5898 citing authors

#	Article	IF	Citations
1	Molecular Models of Hydroxide, Oxyhydroxide, and Clay Phases and the Development of a General Force Field. Journal of Physical Chemistry B, 2004, 108, 1255-1266.	2.6	2,281
2	Molecular Controls on Kaolinite Surface Charge. Journal of Colloid and Interface Science, 1996, 183, 356-364.	9.4	273
3	Molecular models and simulations of layered materials. Journal of Materials Chemistry, 2009, 19, 2470.	6.7	244
4	Molecular Simulation of Carbon Dioxide Capture by Montmorillonite Using an Accurate and Flexible Force Field. Journal of Physical Chemistry C, 2012, 116, 13079-13091.	3.1	234
5	Structure, Energetics, and Dynamics of Water Adsorbed on the Muscovite (001) Surface:Â A Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2005, 109, 15893-15905.	2.6	202
6	Swelling Properties of Montmorillonite and Beidellite Clay Minerals from Molecular Simulation: Comparison of Temperature, Interlayer Cation, and Charge Location Effects. Journal of Physical Chemistry C, 2015, 119, 20880-20891.	3.1	184
7	Molecular Dynamics Modeling of Ion Adsorption to the Basal Surfaces of Kaolinite. Journal of Physical Chemistry C, 2007, 111, 6753-6762.	3.1	165
8	Water Structure and Aqueous Uranyl(VI) Adsorption Equilibria onto External Surfaces of Beidellite, Montmorillonite, and Pyrophyllite:â€‰ Results from Molecular Simulations. Environmental Science & Technology, 2006, 40, 3865-3871.	10.0	138
9	<I>Ab initio</I> determination of edge surface structures for dioctahedral 2:1 phyllosilicates: implications for acid-base for reactivity. Clays and Clay Minerals, 2003, 51, 359-371.	1.3	135
10	Molecular dynamics simulation of uranyl(vi) adsorption equilibria onto an external montmorillonite surface. Physical Chemistry Chemical Physics, 2005, 7, 3580.	2.8	132
11	Molecular Simulation of Carbon Dioxide, Brine, and Clay Mineral Interactions and Determination of Contact Angles. Environmental Science & Technology, 2014, 48, 2035-2042.	10.0	124
12	133Cs NMR and XPS investigation of cesium adsorbed on clay minerals and related phases. Geochimica Et Cosmochimica Acta, 1996, 60, 1041-1052.	3.9	116
13	133Cs NMR study of cesium on the surfaces of kaolinite and illite. Geochimica Et Cosmochimica Acta, 1996, 60, 4059-4074.	3.9	111
14	Molecular Dynamics Simulations of Carbon Dioxide Intercalation in Hydrated Na-Montmorillonite. Journal of Physical Chemistry C, 2013, 117, 11028-11039.	3.1	107
15	Molecular modeling of the structure and dynamics of the interlayer and surface species of mixed-metal layered hydroxides: Chloride and water in hydrocalumite (Friedelâ€™s salt). American Mineralogist, 2000, 85, 1046-1052.	1.9	101
16	Molecular Models for the Intercalation of Methane Hydrate Complexes in Montmorillonite Clay. Journal of Physical Chemistry B, 2004, 108, 15141-15149.	2.6	101
17	A shell model for the simulation of rhombohedral carbonate minerals and their point defects. American Mineralogist, 2000, 85, 217-224.	1.9	95
18	Advances in Clayff Molecular Simulation of Layered and Nanoporous Materials and Their Aqueous Interfaces. Journal of Physical Chemistry C, 2021, 125, 17573-17589.	3.1	95

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19	Structure of Hydrated Gibbsite and Brucite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metalâ€“Oâ€“H Angle Bending Terms. Journal of Physical Chemistry C, 2017, 121, 14757-14771.	3.1	91
20	Structure of the (101Ì„4) surfaces of calcite, dolomite and magnesite under wet and dry conditions. Physical Chemistry Chemical Physics, 2001, 3, 839-844.	2.8	83
21	Molecular Simulation of Structure and Diffusion at Smectiteâ€“Water Interfaces: Using Expanded Clay Interlayers as Model Nanopores. Journal of Physical Chemistry C, 2015, 119, 17126-17136.	3.1	83
22	All-atom ab initio energy minimization of the kaolinite crystal structure. American Mineralogist, 1997, 82, 657-662.	1.9	82
23	Molecular models of a hydrated calcite mineral surface. Geochimica Et Cosmochimica Acta, 2007, 71, 5876-5887.	3.9	79
24	Molecular Dynamics Simulation of Diffusion and Electrical Conductivity in Montmorillonite Interlayers. Journal of Physical Chemistry C, 2016, 120, 1640-1649.	3.1	75
25	Synthesis, structure, and molecular modeling of a titanoniobate isopolyanion. Journal of Solid State Chemistry, 2003, 176, 111-119.	2.9	74
26	An ab Initio and Classical Molecular Dynamics Investigation of the Structural and Vibrational Properties of Talc and Pyrophyllite. Journal of Physical Chemistry C, 2007, 111, 12752-12759.	3.1	73
27	Diffusion of Ca and Mg in calcite. American Mineralogist, 1999, 84, 1392-1399.	1.9	72
28	Molecular Dynamics Simulations of Structural and Mechanical Properties of Muscovite: Pressure and Temperature Effects. Journal of Physical Chemistry C, 2012, 116, 15099-15107.	3.1	65
29	Magnesium self-diffusion in orthoenstatite. Contributions To Mineralogy and Petrology, 1998, 130, 390-396.	3.1	62
30	Crystal growth and the formation of chemical zoning in garnets. Contributions To Mineralogy and Petrology, 1982, 79, 187-200.	3.1	61
31	Adsorption of Aqueous Crude Oil Components on the Basal Surfaces of Clay Minerals: Molecular Simulations Including Salinity and Temperature Effects. Journal of Physical Chemistry C, 2017, 121, 22773-22786.	3.1	61
32	Structure of Hydrated Kaolinite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metalâ€“Oâ€“H Angle Bending Terms. Journal of Physical Chemistry C, 2019, 123, 11628-11638.	3.1	61
33	Molecular Models of Cesium and Rubidium Adsorption on Weathered Micaceous Minerals. Journal of Physical Chemistry A, 2015, 119, 5691-5700.	2.5	60
34	The structure and properties of binary zinc phosphate glasses studied by molecular dynamics simulations. Journal of Non-Crystalline Solids, 2003, 316, 261-272.	3.1	59
35	Analysis of Molecular Clusters in Simulations of Lithium-Ion Battery Electrolytes. Journal of Physical Chemistry C, 2013, 117, 24673-24684.	3.1	59
36	An interatomic potential model for carbonates allowing for polarization effects. Physics and Chemistry of Minerals, 2003, 30, 416-424.	0.8	58

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37	Molecular models of alginic acid: Interactions with calcium ions and calcite surfaces. Geochimica Et Cosmochimica Acta, 2006, 70, 3508-3532.	3.9	57
38	Gibbsite growth kinetics on gibbsite, kaolinite, and muscovite substrates: atomic force microscopy evidence for epitaxy and an assessment of reactive surface area. Geochimica Et Cosmochimica Acta, 1999, 63, 2337-2351.	3.9	56
39	Nanoconfined Water in Magnesium-Rich 2:1 Phyllosilicates. Journal of the American Chemical Society, 2009, 131, 8155-8162.	13.7	55
40	Ca self-diffusion in grossular garnet. American Mineralogist, 1996, 81, 448-451.	1.9	50
41	Vibrational Spectra of Methane Clathrate Hydrates from Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2006, 110, 6428-6431.	2.6	50
42	Chemical and Hydrodynamic Mechanisms for Long-Term Geological Carbon Storage. Journal of Physical Chemistry C, 2014, 118, 15103-15113.	3.1	50
43	Modeling the Polymerization Process for Geopolymer Synthesis through Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 6760-6773.	3.1	49
44	Molecular Simulations of Carbon Dioxide and Water: Cation Solvation. Environmental Science & Technology, 2013, 47, 87-94.	10.0	47
45	Implementation of a Morse potential to model hydroxyl behavior in phyllosilicates. Journal of Chemical Physics, 2009, 130, 134713.	3.0	45
46	Methylene Blue Adsorption on the Basal Surfaces of Kaolinite: Structure and Thermodynamics from Quantum and Classical Molecular Simulation. Clays and Clay Minerals, 2015, 63, 185-198.	1.3	45
47	Dissolution kinetics of experimentally shocked silicate minerals. Chemical Geology, 1989, 78, 229-244.	3.3	44
48	Atomistic models of carbonate minerals: Bulk and surface structures, defects, and diffusion. Molecular Simulation, 2002, 28, 475-495.	2.0	41
49	Molecular Dynamics Simulation of Resin Adsorption at Kaolinite Edge Sites: Effect of Surface Deprotonation on Interfacial Structure. Journal of Physical Chemistry C, 2017, 121, 22787-22796.	3.1	40
50	Inelastic Neutron Scattering and Molecular Simulation of the Dynamics of Interlayer Water in Smectite Clay Minerals. Journal of Physical Chemistry C, 2015, 119, 28005-28019.	3.1	39
51	Molecular dynamics studies of nanoconfined water in clinoptilolite and heulandite zeolites. Physical Chemistry Chemical Physics, 2008, 10, 800-807.	2.8	38
52	Vibrational Analysis of Brucite Surfaces and the Development of an Improved Force Field for Molecular Simulation of Interfaces. Journal of Physical Chemistry C, 2014, 118, 7946-7953.	3.1	37
53	Molecular models of birnessite and related hydrated layered minerals. American Mineralogist, 2012, 97, 1505-1514.	1.9	36
54	Molecular dynamics simulations of uranyl adsorption and structure on the basal surface of muscovite. Molecular Simulation, 2014, 40, 610-617.	2.0	36

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55	Mineral dissolution and precipitation during CO2 injection at the Frio-I Brine Pilot: Geochemical modeling and uncertainty analysis. International Journal of Greenhouse Gas Control, 2016, 44, 166-174.	4.6	35
56	Mg self-diffusion in pyrope garnet. American Mineralogist, 1995, 80, 483-490.	1.9	34
57	Vibrational spectroscopy of brucite: A molecular simulation investigation. American Mineralogist, 2006, 91, 1188-1196.	1.9	34
58	Incoherent Inelastic Neutron Scattering Studies of Nanoconfined Water in Clinoptilolite and Heulandite Zeolites. Journal of Physical Chemistry C, 2008, 112, 13629-13634.	3.1	34
59	Molecular simulations of metal adsorption to bacterial surfaces. Geochimica Et Cosmochimica Acta, 2006, 70, 5075-5088.	3.9	32
60	Molecular Modeling of the Tributyl Phosphate Complex of Europium Nitrate in the Clay Hectorite. Journal of Physical Chemistry A, 1998, 102, 6722-6729.	2.5	31
61	Water and Halide Adsorption to Corrosion Surfaces: Molecular Simulations of Atmospheric Interactions with Aluminum Oxyhydroxide and Gold. Chemistry of Materials, 2008, 20, 4682-4693.	6.7	31
62	Interactions of Kaolin Minerals in the Environment. Elements, 2014, 10, 195-200.	0.5	30
63	Molecular Simulations of Anhydrous Na6[Al6Si6O24] Sodalite. Chemistry of Materials, 2004, 16, 2121-2133.	6.7	28
64	Characterization of Adsorption Sites on Aggregate Soil Samples Using Synchrotron X-ray Computerized Microtomography. Environmental Science & Technology, 2005, 39, 2679-2685.	10.0	27
65	Evaluation of the elasticity normal to the basal plane of non-expandable 2:1 phyllosilicate minerals by nanoindentation. American Mineralogist, 2010, 95, 863-869.	1.9	27
66	Linear Free Energy Relationships between Dissolution Rates and Molecular Modeling Energies of Rhombohedral Carbonates. Langmuir, 2004, 20, 2938-2946.	3.5	26
67	Implications of magma chamber dynamics for Soretâ€related fractionation. Journal of Geophysical Research, 1986, 91, 11451-11461.	3.3	22
68	Molecular dynamics simulations of the lithium coordination environment in phosphate glasses. Physical Chemistry Chemical Physics, 2000, 2, 4427-4432.	2.8	21
69	A Molecular Basis for Advanced Materials in Water Treatment. MRS Bulletin, 2008, 33, 42-47.	3.5	20
70	Molecular Modeling Theory. , 2001, , .		19
71	Time-dependent Soret transport: Applications to brine and magma. Chemical Geology, 1992, 95, 201-212.	3.3	18
72	Cation diffusion in calcite: Determining closure temperatures and the thermal history for the Allan Hills 84001 meteorite. Meteoritics and Planetary Science, 1998, 33, 785-789.	1.6	17

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73	Researchers focus on Earth's response to hypervelocity impacts. Eos, 1996, 77, 197.	0.1	16
74	29 Si MAS NMR relaxation study of shocked Coconino Sandstone from Meteor Crater, Arizona. Physics and Chemistry of Minerals, 1998, 25, 313-317.	0.8	15
75	Impurities and nonstoichiometry in the bulk and on the (101Ì„4) surface of dolomite. Geochimica Et Cosmochimica Acta, 2002, 66, 2541-2546.	3.9	15
76	Effects of thermodynamic ensembles and mineral surfaces on interfacial water structure. Physical Chemistry Chemical Physics, 2012, 14, 1728-1734.	2.8	15
77	Synthesis, Crystal Structure, and Molecular Modeling of a Layered Manganese(II) Phosphate:Â Mn3(PO4)4Â·2(H3NCH2CH2)3NÂ·6(H2O). Chemistry of Materials, 2004, 16, 2068-2075.	6.7	13
78	Role of Water in the Ion Selectivity of Niobate-Based Octahedral Molecular Sieves. Journal of Physical Chemistry C, 2007, 111, 13212-13221.	3.1	13
79	Introduction to a Special Issue on Molecular Computer Simulations of Clays and Clay-Water Interfaces: Recent Progress, Challenges, and Opportunities. Clays and Clay Minerals, 2016, 64, 335-336.	1.3	13
80	Ionic Modeling of Lithium Manganese Spinel Materials for Use in Rechargeable Batteries. Materials Research Society Symposia Proceedings, 1995, 393, 113.	0.1	12
81	Molecular Models of Cesium Sorption on Kaolinite. , 1998, , 383-399.		10
82	Experimental and simulation study of carbon dioxide, brine, and muscovite surface interactions. Journal of Petroleum Science and Engineering, 2017, 155, 78-88.	4.2	10
83	Computational and Spectroscopic Studies of Dichlorofluoroethane Hydrate Structure and Stability. Journal of Physical Chemistry C, 2007, 111, 16787-16795.	3.1	9
84	<I>Ab Initio</I> Study of Hydrogen Storage in Water Clathrates. Journal of Computational and Theoretical Nanoscience, 2010, 7, 2602-2606.	0.4	9
85	Research Activities at U.S. Government Agencies in Subsurface Reactive Transport Modeling. Vadose Zone Journal, 2007, 6, 805-822.	2.2	9
86	Surface Charge and Metal Sorption to Kaolinite. , 1998, , 371-382.		7
87	A thin film approach for producing mineral diffusion couples. Pure and Applied Geophysics, 1993, 141, 631-642.	1.9	6
88	Molecular Dynamics Study of Lithium Diffusion in Lithium-Manganese Spinel Cathode Materials. Materials Research Society Symposia Proceedings, 1997, 496, 109.	0.1	5
89	Power-Law Relaxation of Spin-12 Nuclei in Solids. Journal of Magnetic Resonance Series A, 1994, 106, 116-118.	1.6	3
90	Use of Coupled Passivants and Consolidants on Calcite Mineral Surfaces. Materials Research Society Symposia Proceedings, 1996, 462, 301.	0.1	2

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91	Advances in Molecular Simulation Studies of Clay Minerals. Green Energy and Technology, 2018, , 175-183.	0.6	2
92	NMR spectroscopic examination of shocked sandstone from meteor crater, Arizona. AIP Conference Proceedings, 1994, , .	0.4	1
93	Atomistic Simulations of the (1014) Surface of Carbonate Minerals. Materials Research Society Symposia Proceedings, 2000, 620, 1.	0.1	1
94	Molecular Models of Radionuclide Interaction with Soil Minerals. SSSA Special Publication Series, 0, , 87-109.	0.2	1
95	Monte Carlo and Molecular Dynamics Simulations of Clay Mineral Systems. Green Energy and Technology, 2018, , 147-174.	0.6	1
96	Synthesis, Crystal Structure, and Molecular Modeling of a Layered Manganese(II) Phosphate: Mn3(PO4)4Ã—2 (H3NCH2CH2)3NÃ—6 (H2O).. ChemInform, 2004, 35, no.	0.0	0
97	NMR Spectroscopic Investigations of Surface and Interlayer Species on Minerals, Clays and Other Oxides. , 1997, , 157-168.		0