Jessica M Rimsza

List of Publications by Year
in descending order

48	887	516561 16	501076 28
papers	citations	h-index	g-index

49	49	49	887
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Water Interactions with Nanoporous Silica: Comparison of ReaxFF and ab Initio based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 24803-24816.	1.5	94
2	Development of a ReaxFF Reactive Force Field for NaSiO_x/Water Systems and Its Application to Sodium and Proton Self-Diffusion. Journal of Physical Chemistry C, 2018, 122, 19613-19624.	1.5	63
3	NO_x Adsorption and Optical Detection in Rare Earth Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2019, 11, 43270-43277.	4.0	61
4	Adsorption complexes of copper and copper oxide in the deep eutectic solvent 2:1 ureaâ€“choline chloride. Computational and Theoretical Chemistry, 2012, 987, 57-61.	1.1	52
5	Atomistic computer simulations of water interactions and dissolution of inorganic glasses. Npj Materials Degradation, 2017, 1, .	2.6	51
6	Surface Structure and Stability of Partially Hydroxylated Silica Surfaces. Langmuir, 2017, 33, 3882-3891.	1.6	47
7	Structural and Mechanical Properties of Nanoporous Silica. Journal of the American Ceramic Society, 2014, 97, 772-781.	1.9	40
8	Magnetic Tunability in RE-DOBDC MOFs via NO_x Acid Gas Adsorption. ACS Applied Materials & Interfaces, 2020, 12, 19504-19510.	4.0	39
9	Crack propagation in silica from reactive classical molecular dynamics simulations. Journal of the American Ceramic Society, 2018, 101, 1488-1499.	1.9	36
10	Ab initio Molecular Dynamics Simulations of the Hydroxylation of Nanoporous Silica. Journal of the American Ceramic Society, 2015, 98, 3748-3757.	1.9	34
11	Molecular dynamics simulations of nanoporous organosilicate glasses using Reactive Force Field (ReaxFF). Journal of Non-Crystalline Solids, 2016, 431, 103-111.	1.5	30
12	Chemical Effects on Subcritical Fracture in Silica From Molecular Dynamics Simulations. Journal of Geophysical Research: Solid Earth, 2018, 123, 9341-9354.	1.4	28
13	Tuned Hydrogen Bonding in Rare-Earth Metalâ€“Organic Frameworks for Design of Optical and Electronic Properties: An Exemplar Study of Yâ€“2,5-Dihydroxyterephthalic Acid. ACS Applied Materials & Interfaces, 2020, 12, 4531-4539.	4.0	26
14	Predictive Acid Gas Adsorption in Rare Earth DOBDC Metalâ€“Organic Frameworks via Complementary Cluster and Periodic Structure Models. Journal of Physical Chemistry C, 2020, 124, 26801-26813.	1.5	25
15	Structure and electronic properties of rare earth DOBDC metalâ€“organic-frameworks. Physical Chemistry Chemical Physics, 2019, 21, 23085-23093.	1.3	24
16	Enhanced Sulfur Dioxide Adsorption in UiO-66 Through Crystal Engineering and Chalcogen Bonding. Crystal Growth and Design, 2020, 20, 6139-6146.	1.4	18
17	Prediction of Reactive Nitrous Acid Formation in Rareâ€Earth MOFs via abâ€…initio Molecular Dynamics. Angewandte Chemie - International Edition, 2021, 60, 11514-11522.	7.2	18
18	Kinetically Controlled Linker Binding in Rare Earth-2,5-Dihydroxyterepthalic Acid Metalâ€“Organic Frameworks and Its Predicted Effects on Acid Gas Adsorption. ACS Applied Materials & Interfaces, 2021, 13, 56337-56347.	4.0	15

#	Article	IF	Citations
19	Mechanisms of oxygen plasma damage of amine and methyl terminated organosilicate low-k dielectrics from ab initio molecular dynamics simulations. Journal Physics D: Applied Physics, 2014, 47, 335204.	1.3	14
20	Hydration and Hydroxylation of MgO in Solution: NMR Identification of Proton-Containing Intermediate Phases. ACS Omega, 2019, 4, 1033-1044.	1.6	13
21	Computational and Experimental 1H-NMR Study of Hydrated Mg-Based Minerals. Molecules, 2020, 25, 933.	1.7	13
22	Ar ions and oxygen plasma interactions of amine terminated organosilicate glass: A combined experimental and ab initio simulations study. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2014, 32, .	0.9	12
23	Surface reactions and structural evolution of organosilicate glass under Ar plasma bombardment. Computational Materials Science, 2015, 110, 287-294.	1.4	9
24	Synthesis and characterization of thalliumâ€“salen derivatives for use as underground fluid flow tracers. Dalton Transactions, 2018, 47, 4162-4174.	1.6	9
25	Mechanisms of Silica Fracture in Aqueous Electrolyte Solutions. Frontiers in Materials, 2019, 6, .	1.2	9
26	Energetics and Structure of Agâ€“Water Clusters Formed in Mordenite. Journal of Physical Chemistry C, 2020, 124, 4517-4524.	1.5	9
27	Porous Liquids: Computational Design for Targeted Gas Adsorption. ACS Applied Materials & Interfaces, 2022, 14, 18005-18015.	4.0	9
28	Sensitivity of the strength and toughness of concrete to the properties of the interfacial transition zone. Construction and Building Materials, 2022, 336, 126875.	3.2	9
29	Synthesis, Characterization, and Nanomaterials Generated from 6,6â€²-(((2-Hydroxyethyl)azanediyl)bis(methylene))bis(2,4-di-tert-butylphenol) Modified Group 4 Metal Alkoxides. Inorganic Chemistry, 2018, 57, 11264-11274.	1.9	8
30	Influence of Polymorphs and Local Defect Structures on NMR Parameters of Graphite Fluorides. Journal of Physical Chemistry C, 2021, 125, 2699-2712.	1.5	7
31	Inelastic relaxation in silica via reactive molecular dynamics. Journal of the American Ceramic Society, 2022, 105, 2517-2526.	1.9	7
32	Design Elements for Enhanced Hydrogen Isotope Separations in Barely Porous Organic Cages. ACS Omega, 2022, 7, 7963-7972.	1.6	7
33	Surface Energies and Structure of Saltâ€“Brine Interfaces. Langmuir, 2020, 36, 2482-2491.	1.6	6
34	The Lanthanide Contraction Is a Variable. Inorganic Chemistry, 2022, 61, 6120-6127.	1.9	6
35	Chemical bonding in carborane/aromatic co-polymers: a first-principles analysis of experimental photoemission spectra. Molecular Simulation, 2016, 42, 39-46.	0.9	5
36	Prediction of Reactive Nitrous Acid Formation in Rareâ€Earth MOFs via abâ€…initio Molecular Dynamics. Angewandte Chemie, 2021, 133, 11615-11623.	1.6	5

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37	Water Weakening of Calcium Oxide. Journal of Physical Chemistry C, 2022, 126, 9493-9501.	1.5	5
38	Chemical and electronic structure of composite films deposited by plasma-enhanced chemical vapor deposition from orthocarborane and pyridine source compounds. Journal of Electron Spectroscopy and Related Phenomena, 2018, 223, 21-28.	0.8	3
39	An atomic-scale evaluation of the fracture toughness of silica glass. Journal of Physics Condensed Matter, 2018, 30, 245901.	0.7	3
40	Understanding the effects of polar and non-polar surfactants on the oxidation performance of copper nanoparticles. Journal of Materials Science, 2022, 57, 6167-6181.	1.7	3
41	Fracture mechanisms of sodium silicate glasses. International Journal of Applied Glass Science, 2023, 14, 27-37.	1.0	3
42	Crystal Prediction and Design of Tunable Light Emission in BTBâ€Based Metalâ€Organic Frameworks. Advanced Optical Materials, 2022, 10, .	3.6	3
43	Stability Evaluation of Candidate Precursors for Chemical Vapor Deposition of Hafnium Diboride (HfB₂). ACS Omega, 2021, 6, 11404-11410.	1.6	2
44	Temperature and Pressure Dependence of Saltâ€“Brine Dihedral Angles in the Subsurface. Langmuir, 2021, 37, 13291-13299.	1.6	2
45	Synthesis, characterization, and computational modeling of 6,6'-(((2-hydroxyethyl)azanediyl)bis(methylene))bis(2,4-di-tert-butylphenol) modified group 4 metal alkoxides. Journal of Coordination Chemistry, 2020, 73, 1389-1406.	0.8	1
46	The role of precursor decomposition in the formation of samarium doped ceria nanoparticles via solid-state microwave synthesis. SN Applied Sciences, 2021, 3, 1.	1.5	1
47	Organosilicate glass dielectric films with backbone carbon: Enhanced resistance to carbon loss in plasma environments. , 2014, , .		0
48	Influence of Al location on formation of silver clusters in mordenite. Microporous and Mesoporous Materials, 2021, 327, 111401.	2.2	0