

Daniel H Robertson

List of Publications by Year in descending order

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32
papers

4,895
citations

361296

20
h-index

477173

29
g-index

34
all docs

34
docs citations

34
times ranked

5371
citing authors

#	ARTICLE	IF	CITATIONS
1	Detailed analysis of grid-based molecular docking: A case study of CDOCKER?A CHARMM-based MD docking algorithm. <i>Journal of Computational Chemistry</i> , 2003, 24, 1549-1562.	1.5	1,299
2	Energetics of nanoscale graphitic tubules. <i>Physical Review B</i> , 1992, 45, 12592-12595.	1.1	893
3	Helical and rotational symmetries of nanoscale graphitic tubules. <i>Physical Review B</i> , 1993, 47, 5485-5488.	1.1	591
4	Lessons in Molecular Recognition:â€” The Effects of Ligand and Protein Flexibility on Molecular Docking Accuracy. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 45-55.	2.9	358
5	Characteristic Physical Properties and Structural Fragments of Marketed Oral Drugs. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 224-232.	2.9	350
6	Kinomicsâ€”structural biology and chemogenomics of kinase inhibitors and targets. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2004, 1697, 243-257.	1.1	168
7	Kinomics: characterizing the therapeutically validated kinase space. <i>Drug Discovery Today</i> , 2005, 10, 839-846.	3.2	164
8	Detonations at nanometer resolution using molecular dynamics. <i>Physical Review Letters</i> , 1993, 70, 2174-2177.	2.9	137
9	Properties of fullerene nanotubes. <i>Journal of Physics and Chemistry of Solids</i> , 1993, 54, 1835-1840.	1.9	136
10	Predicting the early risk of chronic kidney disease in patients with diabetes using real-world data. <i>Nature Medicine</i> , 2019, 25, 57-59.	15.2	120
11	On the way to fullerenes: molecular dynamics study of the curling and closure of graphitic ribbons. <i>The Journal of Physical Chemistry</i> , 1992, 96, 6133-6135.	2.9	116
12	Electrochemical Reduction of Nitrate and Nitrite in Concentrated Sodium Hydroxide at Platinum and Nickel Electrodes. <i>Journal of the Electrochemical Society</i> , 1988, 135, 1154-1158.	1.3	88
13	Structure-based design of a new class of highly selective aminoimidazo[1,2-a]pyridine-based inhibitors of cyclin dependent kinases. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 1943-1947.	1.0	86
14	Split shock waves from molecular dynamics. <i>Physical Review Letters</i> , 1991, 67, 3132-3135.	2.9	57
15	Properties of Capped Nanotubes When Used as SPM Tips. <i>Journal of Physical Chemistry B</i> , 1997, 101, 9682-9685.	1.2	56
16	Molecular-dynamics simulations of void collapse in shocked model-molecular solids. <i>Physical Review B</i> , 1994, 49, 14859-14864.	1.1	55
17	Identifying agonistic and antagonistic mechanisms operative at the GABA receptor. <i>Journal of Neuroscience Research</i> , 1995, 42, 666-673.	1.3	32
18	Temperature-Dependent Fusion of Colliding C60 Fullerenes from Molecular Dynamics Simulations. <i>The Journal of Physical Chemistry</i> , 1995, 99, 15721-15724.	2.9	28

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19	A combined simulated annealing and quasi-Newton-like conjugate-gradient method for determining the structure of mixed argon-xenon clusters. <i>Computers & Chemistry</i> , 1990, 14, 305-311.	1.2	27
20	Group-IV covalent clusters: Si ₄₅ and C ₄₄ versus Si ₄₄ and C ₄₅ . <i>Physical Review B</i> , 1991, 44, 3479-3482.	1.1	26
21	Determination of the structure of mixed argon-xenon clusters using a finite-temperature, lattice-based Monte Carlo method. <i>Journal of Chemical Physics</i> , 1989, 90, 3221-3229.	1.2	19
22	Glycine and GABA receptors: Molecular mechanisms controlling chloride ion flux. , 1996, 43, 372-381.		16
23	Study of enzyme-catalyzed reactions in organic solvents using multiple linear regression. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 1999, 7, 273-282.	1.8	14
24	Predicting onset of complications from diabetes: a graph based approach. <i>Applied Network Science</i> , 2018, 3, 48.	0.8	14
25	A Novel Open Access Web Portal for Integrating Mechanistic and Toxicogenomic Study Results. <i>Toxicological Sciences</i> , 2019, 170, 296-309.	1.4	13
26	Dissociative phase transitions from hypervelocity impacts. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1992, 188, 357-366.	1.2	11
27	Chemistry and phase transitions from hypervelocity impacts. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 129-137.	1.0	8
28	Computational Chemistry for the Inorganic Curriculum. <i>Journal of Chemical Education</i> , 1996, 73, 105.	1.1	6
29	Higher-order Networks of Diabetes Comorbidities: Disease Trajectories that Matter. , 2020, , .		5
30	The transition temperatures and dynamics for the argon-xenon N=7 mixed cluster series. <i>Journal of Chemical Physics</i> , 1990, 93, 702-710.	1.2	1
31	AB INITIO MO CALCULATION STUDIES FOR SEVERAL NOVEL ENTRIES TO TROPANE COMPOUNDS. <i>Journal of Theoretical and Computational Chemistry</i> , 2004, 03, 305-323.	1.8	1
32	Utilization of electronic health records for the assessment of adiponectin receptor autoantibodies during the progression of cardio-metabolic comorbidities. , 2020, 1, 17-27.		0