Karl N Kirschner

List of Publications by Year
in descending order

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54	3,444	257357 24	175177 52
papers	citations	h-index	g-index

54	54	54	5158
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Optimizing Lennard-Jones parameters by coupling single molecule and ensemble target data. Computer Physics Communications, 2022, 274, 108285.	3.0	1
2	Molecular Dynamics in the Energy Sector: Experiment and Modeling of the CO₂/CH₄ Mixture. Journal of Chemical & Engineering Data, 2020, 65, 1117-1123.	1.0	4
3	Teaching Technical Journalism with an Engineering Foundation. , 2020, , .		0
4	Interaction of natural flavonoid eriocitrin with Î²-cyclodextrin and hydroxypropyl-Î²-cyclodextrin: an NMR and molecular dynamics investigation. New Journal of Chemistry, 2020, 44, 16431-16441.	1.4	14
5	The performance of Dunning, Jensen, and Karlsruhe basis sets on computing relative energies and geometries. Soft Materials, 2020, 18, 200-214.	0.8	10
6	ACPYPE update for nonuniform 1â€“4 scale factors: Conversion of the GLYCAM06 force field from AMBER to GROMACS. SoftwareX, 2019, 10, 100241.	1.2	41
7	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. Journal of Chemical Theory and Computation, 2019, 15, 3854-3867.	2.3	25
8	Selective targeting of NAMPT by KPT-9274 in acute myeloid leukemia. Blood Advances, 2019, 3, 242-255.	2.5	38
9	Small Alcohols Revisited: CCSD(T) Relative Potential Energies for the Minima, First- and Second-Order Saddle Points, and Torsion-Coupled Surfaces. ACS Omega, 2018, 3, 419-432.	1.6	13
10	Relative electronic and free energies of octane's unique conformations. Molecular Physics, 2017, 115, 1155-1165.	0.8	6
11	Structural analysis of human glycoprotein butyrylcholinesterase using atomistic molecular dynamics: The importance of glycosylation site ASN241. PLoS ONE, 2017, 12, e0187994.	1.1	15
12	Molecular Dynamics Simulation of Membrane Free Energy Profiles Using Accurate Force Field for Ionic Liquids. , 2017, , 265-284.		0
13	Optimized atomistic force fields for aqueous solutions of Magnesium and Calcium Chloride: Analysis, achievements and limitations. European Physical Journal: Special Topics, 2016, 225, 1391-1409.	1.2	10
14	Optimizing Molecular Models Through Force-Field Parameterization via the Efficient Combination of Modular Program Packages. Molecular Modeling and Simulation, 2016, , 53-77.	0.2	11
15	Visualizing potential energy curves and conformations on ultra high-resolution display walls. Journal of Molecular Graphics and Modelling, 2015, 62, 174-180.	1.3	4
16	Structureâ€“activity relationships of thiostrepton derivatives: implications for rational drug design. Journal of Computer-Aided Molecular Design, 2014, 28, 1205-1215.	1.3	9
17	Principal component and clustering analysis on molecular dynamics data of the ribosomal L11Â·23S subdomain. Journal of Molecular Modeling, 2013, 19, 539-549.	0.8	97
18	Structure and thermodynamics of H3O+(H2O)8 clusters: A combined molecular dynamics and quantum mechanics approach. Computational and Theoretical Chemistry, 2013, 1021, 240-248.	1.1	13

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19	Wolf₂Pack â€“ Portal Based Atomistic Force-Field Development. Journal of Chemical Information and Modeling, 2013, 53, 802-808.	2.5	11
20	Quantum Mechanical Study of Sulfuric Acid Hydration: Atmospheric Implications. Journal of Physical Chemistry A, 2012, 116, 2209-2224.	1.1	111
21	A Glycam-Based Force Field for Simulations of Lipopolysaccharide Membranes: Parametrization and Validation. Journal of Chemical Theory and Computation, 2012, 8, 4719-4731.	2.3	96
22	Influence of thiostrepton binding on the ribosomal GTPase associated region characterized by molecular dynamics simulation. Bioorganic and Medicinal Chemistry, 2012, 20, 7194-7205.	1.4	10
23	Liquidâ€“liquid equilibria of dipropylene glycol dimethyl ether and water by molecular dynamics. Fluid Phase Equilibria, 2011, 310, 25-31.	1.4	10
24	NMR Structures of Thiostrepton Derivatives for Characterization of the Ribosomal Binding Site. Angewandte Chemie - International Edition, 2011, 50, 3308-3312.	7.2	33
25	A modern workflow for force-field development â€“ Bridging quantum mechanics and atomistic computational models. Computer Physics Communications, 2011, 182, 2184-2191.	3.0	21
26	Multi-objective optimisation on the basis of random models for ethylene oxide. Molecular Simulation, 2010, 36, 1208-1218.	0.9	5
27	Atomistic simulations of isotactic and atactic poly(methyl methacrylate) melts: exploring the backbone conformational space. Molecular Simulation, 2010, 36, 1253-1264.	0.9	11
28	Ramachandranâ€type plots for glycosidic linkages: Examples from molecular dynamic simulations using the Glycam06 force field. Journal of Computational Chemistry, 2009, 30, 910-921.	1.5	38
29	GLYCAM06: A generalizable biomolecular force field. Carbohydrates. Journal of Computational Chemistry, 2008, 29, 622-655.	1.5	1,778
30	[{2,6â€(Me₂NCH₂)₂C₆H₃}Sn]₂: An Intramolecularly Coordinated Diorganodistannyne. Angewandte Chemie - International Edition, 2008, 47, 1650-1653.	7.2	90
31	Binding free energy calculation for duocarmycin/DNA complex based on the QPLD-derived partial charge model. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 542-545.	1.0	14
32	The Limitations of Certain Density Functionals in Modeling Neutral Water Clusters. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry, 2008, 38, 32-39.	0.6	45
33	Thermodynamics of the Hydroxyl Radical Addition to Isoprene. Journal of Physical Chemistry A, 2008, 112, 7064-7071.	1.1	31
34	Hydration of OCS with One to Four Water Molecules in Atmospheric and Laboratory Conditions. Journal of Physical Chemistry A, 2008, 112, 4490-4495.	1.1	27
35	Efficient and Accurate Characterization of the Bergman Cyclization for Several Enediynes Including an Expanded Substructure of Esperamicin A1. Journal of Physical Chemistry B, 2008, 112, 16917-16934.	1.2	18
36	In search of CS2(H2O)n=1â€“4 clusters. Journal of Chemical Physics, 2007, 126, 154320.	1.2	20

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37	Computational Design and Experimental Discovery of an Antiestrogenic Peptide Derived from Î±-Fetoprotein. Journal of the American Chemical Society, 2007, 129, 6263-6268.	6.6	26
38	Calculating Interaction Energies Using First Principle Theories: Consideration of Basis Set Superposition Error and Fragment Relaxation. Journal of Chemical Education, 2007, 84, 1225.	1.1	32
39	The search for low energy conformational families of small peptides: Searching for active conformations of small peptides in the absence of a known receptor. International Journal of Quantum Chemistry, 2007, 107, 3001-3012.	1.0	12
40	Reconciling solvent effects on rotamer populations in carbohydrates Â— A joint MD and NMR analysis. Canadian Journal of Chemistry, 2006, 84, 569-579.	0.6	47
41	Prediction of Accurate Anharmonic Experimental Vibrational Frequencies for Water Clusters, (H2O)n, n = 2â^'5. Journal of Physical Chemistry A, 2006, 110, 303-309.	1.1	99
42	Exploration of the Potential Energy Surfaces, Prediction of Atmospheric Concentrations, and Prediction of Vibrational Spectra for the HO2Â·Â·Â·(H2O)n(n= 1â^'2) Hydrogen Bonded Complexes. Journal of Physical Chemistry A, 2006, 110, 3686-3691.	1.1	39
43	Ortho Effect in the Bergman Cyclization:â€‰ Electronic and Steric Effects in Hydrogen Abstraction by 1-Substituted Naphthalene 5,8-Diradicals. Journal of Physical Chemistry A, 2006, 110, 2517-2526.	1.1	48
44	Do Hydroxyl Radicalâ^'Water Clusters, OH(H2O)n,n= 1â^'5, Exist in the Atmosphere?. Journal of Physical Chemistry A, 2006, 110, 13283-13289.	1.1	93
45	Incorporation of Carbohydrates into Macromolecular Force Fields: Development and Validation. ACS Symposium Series, 2006, , 235-257.	0.5	10
46	CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. International Journal of Quantum Chemistry, 2006, 106, 3122-3128.	1.0	29
47	Pople's Gaussian-3 model chemistry applied to an investigation of (H2O)8water clusters. International Journal of Quantum Chemistry, 2005, 102, 565-572.	1.0	38
48	Global Search for Minimum Energy (H2O)n Clusters, n = 3â^'5. Journal of Physical Chemistry A, 2005, 109, 6773-6778.	1.1	89
49	Quantum Mechanical Study of the Nonbonded Forces in Waterâ^'Methanol Complexes. Journal of Physical Chemistry A, 2001, 105, 4150-4155.	1.1	101
50	Density functional and ab initio studies on N -acetyl-duocarmycin SA: insight into its DNA interaction properties. Bioorganic and Medicinal Chemistry, 2000, 8, 329-335.	1.4	7
51	Use of the Supermolecule Approach To Model the Syn and Anti Conformations of Solvated Cyclic 3â€˜,5â€˜-Adenosine Monophosphate. The Journal of Physical Chemistry, 1996, 100, 3293-3298.	2.9	21
52	Quantum mechanical investigation of cyclic 3â€²,5â€²-adenosine monophosphate, the second hormonal messenger. Computational and Theoretical Chemistry, 1996, 362, 297-304.	1.5	9
53	Quantum-Mechanical investigation of large water clusters. International Journal of Quantum Chemistry, 1994, 52, 349-360.	1.0	29
54	Modeling of magic water clusters (H2O)20 and (H2O)21H+ with the PM3 quantum-mechanical method. Journal of Computational Chemistry, 1993, 14, 1326-1332.	1.5	35