# Karl N Kirschner

List of Publications by Year
in descending order



| 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 | GLYCAM06: A generalizable biomolecular force field. Carbohydrates. Journal of Computational Chemistry, 2008, 29, 622-655. | 1.5 | 1,778 |
| 2 | Quantum Mechanical Study of Sulfuric Acid Hydration: Atmospheric Implications. Journal of Physical Chemistry A, 2012, 116, 2209-2224. | 1.1 | 111 |
| 3 | Quantum Mechanical Study of the Nonbonded Forces in Waterâ˜Methanol Complexes. Journal of Physical Chemistry A, 2001, 105, 4150-4155. | 1.1 | 101 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | 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 |
| 8 | [{2,6â€(Me<sub>2</sub>NCH<sub>2</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>}Sn]<sub>2</sub>: An Intramolecularly Coordinated Diorganodistannyne. Angewandte Chemie - International Edition, 2008, 47, 1650-1653. | 7.2 | 90 |
| 9 | Global Search for Minimum Energy (H2O)n Clusters, n = 3â˜5. Journal of Physical Chemistry A, 2005, 109, 6773-6778. | 1.1 | 89 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | Selective targeting of NAMPT by KPT-9274 in acute myeloid leukemia. Blood Advances, 2019, 3, 242-255. | 2.5 | 38 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | NMR Structures of Thiostrepton Derivatives for Characterization of the Ribosomal Binding Site. Angewandte Chemie - International Edition, 2011, 50, 3308-3312. | 7.2 | 33 |
| 20 | 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 |
| 21 | Thermodynamics of the Hydroxyl Radical Addition to Isoprene. Journal of Physical Chemistry A, 2008, 112, 7064-7071. | 1.1 | 31 |
| 22 | Quantum-Mechanical investigation of large water clusters. International Journal of Quantum Chemistry, 1994, 52, 349-360. | 1.0 | 29 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | In search of CS2(H2O)n=1â€“4 clusters. Journal of Chemical Physics, 2007, 126, 154320. | 1.2 | 20 |
| 30 | 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 |
| 31 | Structural analysis of human glycoprotein butyrylcholinesterase using atomistic molecular dynamics: The importance of glycosylation site ASN241. PLoS ONE, 2017, 12, e0187994. | 1.1 | 15 |
| 32 | 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 |
| 33 | 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 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Atomistic simulations of isotactic and atactic poly(methyl methacrylate) melts: exploring the backbone conformational space. Molecular Simulation, 2010, 36, 1253-1264. | 0.9 | 11 |
| 38 | Wolf<sub>2</sub>Pack â€“ Portal Based Atomistic Force-Field Development. Journal of Chemical Information and Modeling, 2013, 53, 802-808. | 2.5 | 11 |
| 39 | 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 |
| 40 | Incorporation of Carbohydrates into Macromolecular Force Fields: Development and Validation. ACS Symposium Series, 2006, , 235-257. | 0.5 | 10 |
| 41 | Liquidâ€“liquid equilibria of dipropylene glycol dimethyl ether and water by molecular dynamics. Fluid Phase Equilibria, 2011, 310, 25-31. | 1.4 | 10 |
| 42 | 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 |
| 43 | 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 |
| 44 | The performance of Dunning, Jensen, and Karlsruhe basis sets on computing relative energies and geometries. Soft Materials, 2020, 18, 200-214. | 0.8 | 10 |
| 45 | 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 |
| 46 | Structureâ€“activity relationships of thiostrepton derivatives: implications for rational drug design. Journal of Computer-Aided Molecular Design, 2014, 28, 1205-1215. | 1.3 | 9 |
| 47 | 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 |
| 48 | Relative electronic and free energies of octane's unique conformations. Molecular Physics, 2017, 115, 1155-1165. | 0.8 | 6 |
| 49 | Multi-objective optimisation on the basis of random models for ethylene oxide. Molecular Simulation, 2010, 36, 1208-1218. | 0.9 | 5 |
| 50 | 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 |
| 51 | Molecular Dynamics in the Energy Sector: Experiment and Modeling of the CO<sub>2</sub>/CH<sub>4</sub> Mixture. Journal of Chemical & Engineering Data, 2020, 65, 1117-1123. | 1.0 | 4 |
| 52 | Optimizing Lennard-Jones parameters by coupling single molecule and ensemble target data. Computer Physics Communications, 2022, 274, 108285. | 3.0 | 1 |
| 53 | Teaching Technical Journalism with an Engineering Foundation. , 2020, , . | | 0 |
| 54 | Molecular Dynamics Simulation of Membrane Free Energy Profiles Using Accurate Force Field for Ionic Liquids. , 2017, , 265-284. | | 0 |