

G Andreïs Cisneros

List of Publications by Year in descending order

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101
papers

3,623
citations

147566

31
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g-index

119
all docs

119
docs citations

119
times ranked

3151
citing authors

#	ARTICLE	IF	CITATIONS
1	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. <i>Chemical Reviews</i> , 2016, 116, 7501-7528.	23.0	314
2	Anisotropic, Polarizable Molecular Mechanics Studies of Inter- and Intramolecular Interactions and Ligand ^π Macromolecule Complexes. A Bottom-Up Strategy. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1960-1986.	2.3	312
3	Classical Electrostatics for Biomolecular Simulations. <i>Chemical Reviews</i> , 2014, 114, 779-814.	23.0	229
4	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. <i>Chemical Science</i> , 2018, 9, 956-972.	3.7	190
5	Towards a force field based on density fitting. <i>Journal of Chemical Physics</i> , 2006, 124, 104101.	1.2	175
6	Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. <i>Journal of Chemical Physics</i> , 2006, 125, 054511.	1.2	169
7	Generalization of the Gaussian electrostatic model: Extension to arbitrary angular momentum, distributed multipoles, and speedup with reciprocal space methods. <i>Journal of Chemical Physics</i> , 2006, 125, 184101.	1.2	100
8	Ab Initio QM/MM Study Shows There Is No General Acid in the Reaction Catalyzed by 4-Oxalocrotonate Tautomerase. <i>Journal of the American Chemical Society</i> , 2003, 125, 10384-10393.	6.6	89
9	Gaussian Multipole Model (GMM). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 190-202.	2.3	79
10	<sc>LICHEM</sc>: A <sc>QM</sc>/<sc>MM</sc> program for simulations with multipolar and polarizable force fields. <i>Journal of Computational Chemistry</i> , 2016, 37, 1019-1029.	1.5	68
11	The Protein Backbone Makes Important Contributions to 4-Oxalocrotonate Tautomerase Enzyme Catalysis: A Understanding from Theory and Experiment. <i>Biochemistry</i> , 2004, 43, 6885-6892.	1.2	64
12	Reaction Mechanism of the β Subunit of E. coli DNA Polymerase III: Insights into Active Site Metal Coordination and Catalytically Significant Residues. <i>Journal of the American Chemical Society</i> , 2009, 131, 1550-1556.	6.6	64
13	GEM*: A Molecular Electronic Density-Based Force Field for Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1361-1365.	2.3	64
14	Mutations along a TET2 active site scaffold stall oxidation at 5-hydroxymethylcytosine. <i>Nature Chemical Biology</i> , 2017, 13, 181-187.	3.9	59
15	<i>Ab Initio</i> QM/MM Calculations Show an Intersystem Crossing in the Hydrogen Abstraction Step in Dealkylation Catalyzed by AlkB. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6410-6420.	1.2	58
16	Application of Gaussian Electrostatic Model (GEM) Distributed Multipoles in the AMOEBA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5072-5080.	2.3	57
17	Concentration-Independent pH Detection with a Luminescent Dimetallic Eu(III)-Based Probe. <i>Journal of the American Chemical Society</i> , 2012, 134, 17372-17375.	6.6	56
18	Intermolecular electrostatic energies using density fitting. <i>Journal of Chemical Physics</i> , 2005, 123, 044109.	1.2	55

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19	Quantum Mechanics/Molecular Mechanics Electrostatic Embedding with Continuous and Discrete Functions. <i>Journal of Physical Chemistry B</i> , 2006, 110, 13682-13684.	1.2	53
20	Simple formulas for improved point-charge electrostatics in classical force fields and hybrid quantum mechanical/molecular mechanical embedding. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1905-1912.	1.0	53
21	Catalytic mechanism of human DNA polymerase β with Mg^{2+} and Mn^{2+} from ab initio quantum mechanical/molecular mechanical studies. <i>DNA Repair</i> , 2008, 7, 1824-1834.	1.3	52
22	Toward a Deeper Understanding of Enzyme Reactions Using the Coupled ELF/NCI Analysis: Application to DNA Repair Enzymes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2156-2160.	2.3	48
23	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. <i>Chemical Science</i> , 2019, 10, 7200-7211.	3.7	45
24	Parallel iterative reaction path optimization in ab initio quantum mechanical/molecular mechanical modeling of enzyme reactions. <i>Journal of Chemical Physics</i> , 2004, 121, 697-706.	1.2	43
25	DFT-steric-based energy decomposition analysis of intermolecular interactions. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	43
26	Development of AMOEBA Force Field for 1,3-Dimethylimidazolium Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7156-7166.	1.2	40
27	QM/MM Simulations with the Gaussian Electrostatic Model: A Density-based Polarizable Potential. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3062-3067.	2.1	37
28	Reaction path determination for quantum mechanical/molecular mechanical modeling of enzyme reactions by combining first order and second order ϵ -chain-of-replicas methods. <i>Journal of Chemical Physics</i> , 2005, 122, 114502.	1.2	36
29	Numerical Fitting of Molecular Properties to Hermite Gaussians. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12049-12056.	1.1	36
30	DFT study of the structural and electronic properties of small Nin ($n=2-4$) clusters. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 847-861.	1.0	35
31	Selectivity and Promiscuity in TET-Mediated Oxidation of 5-Methylcytosine in DNA and RNA. <i>Biochemistry</i> , 2019, 58, 411-421.	1.2	34
32	Alternative Pathway for the Reaction Catalyzed by DNA Dealkylase AlkB from Ab Initio QM/MM Calculations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5136-5148.	2.3	32
33	Synthesis and Reactions of 3d Metal Complexes with the Bulky Alkoxide Ligand $[OC^iBu_2Ph]$. <i>Inorganic Chemistry</i> , 2015, 54, 5624-5633.	1.9	32
34	Novel Alkoxide Cluster Topologies Featuring Rare Seesaw Geometry at Transition Metal Centers. <i>Chemistry - A European Journal</i> , 2013, 19, 12225-12228.	1.7	31
35	Computational Prediction of Residues Involved in Fidelity Checking for DNA Synthesis in DNA Polymerase I. <i>Biochemistry</i> , 2012, 51, 2569-2578.	1.2	29
36	Computational investigation of O_2 diffusion through an intra-molecular tunnel in AlkB; influence of polarization on O_2 transport. <i>Chemical Science</i> , 2017, 8, 6230-6238.	3.7	29

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37	Insight into wild-type and T1372E TET2-mediated 5hmC oxidation using <i>ab initio</i> QM/MM calculations. <i>Chemical Science</i> , 2018, 9, 8433-8445.	3.7	27
38	Development and application of quantum mechanics/molecular mechanics methods with advanced polarizable potentials. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1515.	6.2	27
39	Long-range electrostatic corrections in multipolar/polarizable QM/MM simulations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	24
40	ALKBH7 Variant Related to Prostate Cancer Exhibits Altered Substrate Binding. <i>PLoS Computational Biology</i> , 2017, 13, e1005345.	1.5	24
41	Novel Histone Deacetylase Class IIa Selective Substrate Radiotracers for PET Imaging of Epigenetic Regulation in the Brain. <i>PLoS ONE</i> , 2015, 10, e0133512.	1.1	23
42	Simulations of the water exchange dynamics of lanthanide ions in 1-ethyl-3-methylimidazolium ethyl sulfate ([EMIm][EtSO ₄]) and water. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30323-30333.	1.3	23
43	Current Status of AMOEBA-IL: A Multipolar/Polarizable Force Field for Ionic Liquids. <i>International Journal of Molecular Sciences</i> , 2020, 21, 697.	1.8	23
44	S/G-1: An <i>ab Initio</i> Force-Field Blending Frozen Hermite Gaussian Densities and Distributed Multipoles. Proof of Concept and First Applications to Metal Cations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7598-7612.	1.1	22
45	Theoretical and Experimental Determination on Two Substrates Turned over by 4-Oxalocrotonate Tautomerase. <i>Journal of Physical Chemistry A</i> , 2006, 110, 700-708.	1.1	21
46	A new smoothing function to introduce long-range electrostatic effects in QM/MM calculations. <i>Journal of Chemical Physics</i> , 2015, 143, 044103.	1.2	21
47	Development of an AMOEBA water model using GEM distributed multipoles. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	20
48	Computational and experimental characterization of a pyrrolidinium-based ionic liquid for electrolyte applications. <i>Journal of Chemical Physics</i> , 2017, 147, 161731.	1.2	20
49	Computational Analysis of Ammonia Transfer Along Two Intramolecular Tunnels in <i>Staphylococcus aureus</i> Glutamine-Dependent Amidotransferase (GatCAB). <i>Journal of Physical Chemistry B</i> , 2015, 119, 3669-3677.	1.2	19
50	Computational Simulations of DNA Polymerases: Detailed Insights on Structure/Function/Mechanism from Native Proteins to Cancer Variants. <i>Chemical Research in Toxicology</i> , 2017, 30, 1922-1935.	1.7	19
51	LICHEM 1.1: Recent Improvements and New Capabilities. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3056-3065.	2.3	19
52	Correlation between electron localization and metal ion mutagenicity in DNA synthesis from QM/MM calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11239.	1.3	18
53	Dramatic effect of homoallylic substitution on the rate of palladium-catalyzed diene cycloisomerization. <i>Journal of Organometallic Chemistry</i> , 2003, 687, 498-507.	0.8	15
54	DNArCdb: A database of cancer biomarkers in DNA repair genes that includes variants related to multiple cancer phenotypes. <i>DNA Repair</i> , 2018, 70, 10-17.	1.3	15

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55	DFT study of a model system for the dealkylation step catalyzed by AlkB. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2010, 2, 70-77.	2.2	14
56	Structural and computational dissection of the catalytic mechanism of the inorganic pyrophosphatase from <i>Mycobacterium tuberculosis</i> . <i>Journal of Structural Biology</i> , 2015, 192, 76-87.	1.3	14
57	Molecular dynamics investigation of water-exchange reactions on lanthanide ions in water/1-ethyl-3-methylimidazolium trifluoromethylsulfate ([EMIm][OTf]). <i>Journal of Chemical Physics</i> , 2018, 148, 024503.	1.2	14
58	Single-nucleotide polymorphism of the DNA cytosine deaminase APOBEC3H haplotype I leads to enzyme destabilization and correlates with lung cancer. <i>NAR Cancer</i> , 2020, 2, zcaa023.	1.6	13
59	Computational Study of Putative Residues Involved in DNA Synthesis Fidelity Checking in <i>Thermus aquaticus</i> DNA Polymerase I. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 39-75.	1.0	12
60	Dynamics of the E. coli β^2 -Clamp Dimer Interface and Its Influence on DNA Loading. <i>Biophysical Journal</i> , 2019, 117, 587-601.	0.2	12
61	Development of the Quantum-Inspired SIBFA Many-Body Polarizable Force Field: Enabling Condensed-Phase Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3607-3621.	2.3	12
62	Unraveling Low-Barrier Hydrogen Bonds in Complex Systems with a Simple Quantum Topological Criterion. <i>Chemistry - A European Journal</i> , 2011, 17, 2833-2837.	1.7	11
63	Hypothesis driven single nucleotide polymorphism search (HyDn-SNP-S). <i>DNA Repair</i> , 2013, 12, 733-740.	1.3	11
64	Reduced structural flexibility for an exonuclease deficient DNA polymerase III mutant. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26892-26902.	1.3	11
65	A Many-Body, Fully Polarizable Approach to QM/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7462-7472.	2.3	11
66	Molecular basis for the initiation of DNA primer synthesis. <i>Nature</i> , 2022, 605, 767-773.	13.7	11
67	Further refinements of next-generation force fields "Nonempirical localization of off-centered points in molecules. <i>Canadian Journal of Chemistry</i> , 2013, 91, 804-810.	0.6	10
68	Polarizable ab initio QM/MM Study of the Reaction Mechanism of N-tert-Butyloxycarbonylation of Aniline in [EMIm][BF ₄]. <i>Molecules</i> , 2018, 23, 2830.	1.7	10
69	Homology modeling, molecular dynamics, and site-directed mutagenesis study of AlkB human homolog 1 (ALKBH1). <i>Journal of Molecular Graphics and Modelling</i> , 2014, 54, 123-130.	1.3	9
70	Unfolding Pathways of Hen Egg-White Lysozyme in Ethanol. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3267-3271.	1.2	9
71	Electrostatics Interactions in Classical Simulations. <i>Methods in Molecular Biology</i> , 2013, 924, 243-270.	0.4	8
72	Energetic Materials Trends in 5- and 6-Membered Cyclic Peroxides Containing Hydroperoxy and Hydroxy Substituents. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5036-5043.	1.0	8

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73	Characterization of Nine Cancer-Associated Variants in Human DNA Polymerase β . <i>Chemical Research in Toxicology</i> , 2018, 31, 697-711.	1.7	8
74	Multipolar/polarizable molecular dynamics simulations of Liquid-liquid extraction of benzene from hydrocarbons using ionic liquids. <i>Journal of Molecular Liquids</i> , 2019, 296, 111846.	2.3	8
75	Catalytic Mechanism of 4-Oxalocrotonate Tautomerase: Significances of Protein-Protein Interactions on Proton Transfer Pathways. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6889-6897.	1.2	7
76	Characterization of tunnel mutants reveals a catalytic step in ammonia delivery by an aminoacyl-tRNA amidotransferase. <i>FEBS Letters</i> , 2016, 590, 3122-3132.	1.3	7
77	Ewald-based methods for Gaussian integral evaluation: application to a new parameterization of GEM*. <i>Journal of Molecular Modeling</i> , 2019, 25, 307.	0.8	7
78	Impact of Remdesivir Incorporation along the Primer Strand on SARS-CoV-2 RNA-Dependent RNA Polymerase. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2456-2465.	2.5	7
79	The Kinase Activity of the <i>Helicobacter pylori</i> Asp-tRNA ^{Asn} /Glu-tRNA ^{Gln} Amidotransferase Is Sensitive to Distal Mutations in Its Putative Ammonia Tunnel. <i>Biochemistry</i> , 2012, 51, 273-285.	1.2	6
80	Exploring the structural determinants of selective phosphopeptide recognition using bivalent metal-coordination complexes. <i>MedChemComm</i> , 2013, 4, 289-292.	3.5	6
81	Bulky Lesion Bypass Requires Dpo4 Binding in Distinct Conformations. <i>Scientific Reports</i> , 2017, 7, 17383.	1.6	6
82	Ground State Destabilization in Uracil DNA Glycosylase: Let's Not Forget α -Tautomeric Strain in Substrates. <i>Journal of the American Chemical Society</i> , 2019, 141, 13739-13743.	6.6	6
83	Computational investigations of selected enzymes from two iron and α -ketoglutarate-dependent families. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22227-22240.	1.3	6
84	Combining Evolutionary Conservation and Quantum Topological Analyses To Determine Quantum Mechanics Subsystems for Biomolecular Quantum Mechanics/Molecular Mechanics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4524-4537.	2.3	6
85	Efficient optimization of van der Waals parameters from bulk properties. <i>Journal of Computational Chemistry</i> , 2013, 34, 2313-2319.	1.5	5
86	Investigating carbohydrate based ligands for galectin-3 with docking and molecular dynamics studies. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 71, 211-217.	1.3	5
87	Computational compensatory mutation discovery approach: Predicting a PARP1 variant rescue mutation. <i>Biophysical Journal</i> , 2022, 121, 3663-3673.	0.2	5
88	Computational investigation of non-covalent interactions in 1-butyl 3-methylimidazolium/bis(trifluoromethylsulfonyl)imide [bmim][Tf2N] in EMD and NEMD. <i>Journal of Chemical Physics</i> , 2018, 148, 054303.	1.2	4
89	Comparison of DNA and RNA substrate effects on TET2 structure. <i>Advances in Protein Chemistry and Structural Biology</i> , 2019, 117, 91-112.	1.0	4
90	Characterizing Hydrogen-Bond Interactions in Pyrazinetetracarboxamide Complexes: Insights from Experimental and Quantum Topological Analyses. <i>Inorganic Chemistry</i> , 2018, 57, 9775-9778.	1.9	3

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91	Conformational Analysis of Clostridium difficile Toxin B and Its Implications for Substrate Recognition. PLoS ONE, 2012, 7, e41518.	1.1	3
92	Divergence in Dimerization and Activity of Primate APOBEC3C. Journal of Molecular Biology, 2021, 433, 167306.	2.0	3
93	Improvement of the Gaussian Electrostatic Model by separate fitting of Coulomb and exchange-repulsion densities and implementation of a new dispersion term. Journal of Chemical Physics, 2021, 155, 194103.	1.2	3
94	Disruption of Intrinsic Motions as a Mechanism for Enzyme Inhibition. Biophysical Journal, 2013, 105, 494-501.	0.2	2
95	Computational study of pH-responsive lanthanide complexes. International Journal of Quantum Chemistry, 2017, 117, e25406.	1.0	2
96	Structural and electronic analysis of the octarepeat region of prion protein with four Cu ²⁺ by polarizable MD and QM/MM simulations. Physical Chemistry Chemical Physics, 2021, 23, 21568-21578.	1.3	2
97	Electronic Structure Effects Related to the Origin of the Remarkable Near-Infrared Absorption of <i>Blastochloris viridis</i> Light Harvesting 1-Reaction Center Complex. Journal of Chemical Theory and Computation, 2022, 18, 4555-4564.	2.3	2
98	Insights into conformational changes in AlkD bound to DNA with a yatakemycin adduct from computational simulations. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	1
99	Computational Investigation of APOBEC3H Substrate Orientation and Selectivity. Journal of Physical Chemistry B, 2020, 124, 3903-3908.	1.2	1
100	Comparison Of Reaction Barriers In Energy And Free Energy For Enzyme Catalysis. Challenges and Advances in Computational Chemistry and Physics, 2009, , 57-78.	0.6	1
101	Insights into conformational changes in AlkD bound to DNA with a yatakemycin adduct from computational simulations. Theoretical Chemistry Accounts, 2018, 137, .	0.5	0