G AndreÌs Cisneros

List of Publications by Year
in descending order

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101 papers	3,623 citations	147566 31 h-index	143772 57 g-index
119 all docs	119 docs citations	119 times ranked	3151 citing authors

#	Article	IF	Citations
1	Impact of Remdesivir Incorporation along the Primer Strand on SARS-CoV-2 RNA-Dependent RNA Polymerase. Journal of Chemical Information and Modeling, 2022, 62, 2456-2465.	2.5	7
2	Molecular basis for the initiation of DNA primer synthesis. Nature, 2022, 605, 767-773.	13.7	11
3	Development of the Quantum-Inspired SIBFA Many-Body Polarizable Force Field: Enabling Condensed-Phase Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, 18, 3607-3621.	2.3	12
4	Computational compensatory mutation discovery approach: Predicting a PARP1 variant rescue mutation. Biophysical Journal, 2022, 121, 3663-3673.	0.2	5
5	Electronic Structure Effects Related to the Origin of the Remarkable Near-Infrared Absorption of Blastochloris viridisâ€™ Light Harvesting 1-Reaction Center Complex. Journal of Chemical Theory and Computation, 2022, 18, 4555-4564.	2.3	2
6	Computational investigations of selected enzymes from two iron and Î±-ketoglutarate-dependent families. Physical Chemistry Chemical Physics, 2021, 23, 22227-22240.	1.3	6
7	Development and application of quantum mechanics/molecular mechanics methods with advanced polarizable potentials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1515.	6.2	27
8	Structural and electronic analysis of the octarepeat region of prion protein with four Cu2+ by polarizable MD and QM/MM simulations. Physical Chemistry Chemical Physics, 2021, 23, 21568-21578.	1.3	2
9	Combining Evolutionary Conservation and Quantum Topological Analyses To Determine Quantum Mechanics Subsystems for Biomolecular Quantum Mechanics/Molecular Mechanics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 4524-4537.	2.3	6
10	Divergence in Dimerization and Activity of Primate APOBEC3C. Journal of Molecular Biology, 2021, 433, 167306.	2.0	3
11	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
12	Single-nucleotide polymorphism of the DNA cytosine deaminase APOBEC3H haplotype I leads to enzyme destabilization and correlates with lung cancer. NAR Cancer, 2020, 2, zcaa023.	1.6	13
13	A Many-Body, Fully Polarizable Approach to QM/MM Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7462-7472.	2.3	11
14	Computational Investigation of APOBEC3H Substrate Orientation and Selectivity. Journal of Physical Chemistry B, 2020, 124, 3903-3908.	1.2	1
15	Current Status of AMOEBAâ€“IL: A Multipolar/Polarizable Force Field for Ionic Liquids. International Journal of Molecular Sciences, 2020, 21, 697.	1.8	23
16	Comparison of DNA and RNA substrate effects on TET2 structure. Advances in Protein Chemistry and Structural Biology, 2019, 117, 91-112.	1.0	4
17	Multipolar/polarizable molecular dynamics simulations of Liquidâ€“Liquid extraction of benzene from hydrocarbons using ionic liquids. Journal of Molecular Liquids, 2019, 296, 111846.	2.3	8
18	Ground State Destabilization in Uracil DNA Glycosylase: Letâ€™s Not Forget â€œTautomeric Strainâ€• in Substrates. Journal of the American Chemical Society, 2019, 141, 13739-13743.	6.6	6

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19	Ewald-based methods for Gaussian integral evaluation: application to a new parameterization of GEM*. Journal of Molecular Modeling, 2019, 25, 307.	0.8	7
20	Dynamics of the E.Âcoli Î²-Clamp Dimer Interface and Its Influence on DNA Loading. Biophysical Journal, 2019, 117, 587-601.	0.2	12
21	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. Chemical Science, 2019, 10, 7200-7211.	3.7	45
22	LICHEM 1.1: Recent Improvements and New Capabilities. Journal of Chemical Theory and Computation, 2019, 15, 3056-3065.	2.3	19
23	Unfolding Pathways of Hen Egg-White Lysozyme in Ethanol. Journal of Physical Chemistry B, 2019, 123, 3267-3271.	1.2	9
24	Selectivity and Promiscuity in TET-Mediated Oxidation of 5-Methylcytosine in DNA and RNA. Biochemistry, 2019, 58, 411-421.	1.2	34
25	Computational investigation of non-covalent interactions in 1-butyl 3-methylimidazolium/bis(trifluoromethylsulfonyl)imide [bmim][Tf2N] in EMD and NEMD. Journal of Chemical Physics, 2018, 148, 054303.	1.2	4
26	Molecular dynamics investigation of water-exchange reactions on lanthanide ions in water/1-ethyl-3-methylimidazolium trifluoromethylsufate ([EMIm][OTf]). Journal of Chemical Physics, 2018, 148, 024503.	1.2	14
27	Reduced structural flexibility for an exonuclease deficient DNA polymerase III mutant. Physical Chemistry Chemical Physics, 2018, 20, 26892-26902.	1.3	11
28	Polarizable ab initio QM/MM Study of the Reaction Mechanism of N-tert-Butyloxycarbonylation of Aniline in [EMIm][BF4]. Molecules, 2018, 23, 2830.	1.7	10
29	Insight into wild-type and T1372E TET2-mediated 5hmC oxidation using ab initio QM/MM calculations. Chemical Science, 2018, 9, 8433-8445.	3.7	27
30	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
31	QM/MM Simulations with the Gaussian Electrostatic Model: A Density-based Polarizable Potential. Journal of Physical Chemistry Letters, 2018, 9, 3062-3067.	2.1	37
32	DNArCdb: A database of cancer biomarkers in DNA repair genes that includes variants related to multiple cancer phenotypes. DNA Repair, 2018, 70, 10-17.	1.3	15
33	Characterization of Nine Cancer-Associated Variants in Human DNA Polymerase Îº. Chemical Research in Toxicology, 2018, 31, 697-711.	1.7	8
34	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. Chemical Science, 2018, 9, 956-972.	3.7	190
35	Characterizing Hydrogen-Bond Interactions in Pyrazinetetracarboxamide Complexes: Insights from Experimental and Quantum Topological Analyses. Inorganic Chemistry, 2018, 57, 9775-9778.	1.9	3
36	Insights into conformational changes in AlkD bound to DNA with a yatakemycin adduct from computational simulations. Theoretical Chemistry Accounts, 2018, 137, .	0.5	0

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37	Computational study of pHâ€responsive diâ€lanthanide complexes. International Journal of Quantum Chemistry, 2017, 117, e25406.	1.0	2
38	Mutations along a TET2 active site scaffold stall oxidation at 5-hydroxymethylcytosine. Nature Chemical Biology, 2017, 13, 181-187.	3.9	59
39	Computational and experimental characterization of a pyrrolidinium-based ionic liquid for electrolyte applications. Journal of Chemical Physics, 2017, 147, 161731.	1.2	20
40	Computational investigation of O₂diffusion through an intra-molecular tunnel in AlkB; influence of polarization on O₂transport. Chemical Science, 2017, 8, 6230-6238.	3.7	29
41	Computational Simulations of DNA Polymerases: Detailed Insights on Structure/Function/Mechanism from Native Proteins to Cancer Variants. Chemical Research in Toxicology, 2017, 30, 1922-1935.	1.7	19
42	Investigating carbohydrate based ligands for galectin-3 with docking and molecular dynamics studies. Journal of Molecular Graphics and Modelling, 2017, 71, 211-217.	1.3	5
43	Bulky Lesion Bypass Requires Dpo4 Binding in Distinct Conformations. Scientific Reports, 2017, 7, 17383.	1.6	6
44	ALKBH7 Variant Related to Prostate Cancer Exhibits Altered Substrate Binding. PLoS Computational Biology, 2017, 13, e1005345.	1.5	24
45	<scp>LICHEM</scp>: A <scp>QM</scp>/<scp>MM</scp> program for simulations with multipolar and polarizable force fields. Journal of Computational Chemistry, 2016, 37, 1019-1029.	1.5	68
46	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. Chemical Reviews, 2016, 116, 7501-7528.	23.0	314
47	Energetic Materials Trends in 5â€and 6â€Membered Cyclic Peroxides Containing Hydroperoxy and Hydroxy Substituents. European Journal of Inorganic Chemistry, 2016, 2016, 5036-5043.	1.0	8
48	Simulations of the water exchange dynamics of lanthanide ions in 1-ethyl-3-methylimidazolium ethyl sulfate ([EMIm][EtSO₄]) and water. Physical Chemistry Chemical Physics, 2016, 18, 30323-30333.	1.3	23
49	Characterization of tunnel mutants reveals a catalytic step in ammonia delivery by an aminoacylâ€<scp>tRNA</scp> amidotransferase. FEBS Letters, 2016, 590, 3122-3132.	1.3	7
50	Long-range electrostatic corrections in multipolar/polarizable QM/MM simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	24
51	A new smoothing function to introduce long-range electrostatic effects in QM/MM calculations. Journal of Chemical Physics, 2015, 143, 044103.	1.2	21
52	Novel Histone Deacetylase Class IIa Selective Substrate Radiotracers for PET Imaging of Epigenetic Regulation in the Brain. PLoS ONE, 2015, 10, e0133512.	1.1	23
53	Computational Analysis of Ammonia Transfer Along Two Intramolecular Tunnels in Staphylococcus aureus Glutamine-Dependent Amidotransferase (GatCAB). Journal of Physical Chemistry B, 2015, 119, 3669-3677.	1.2	19
54	Synthesis and Reactions of 3d Metal Complexes with the Bulky Alkoxide Ligand [OC^tBu₂Ph]. Inorganic Chemistry, 2015, 54, 5624-5633.	1.9	32

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55	Development of an AMOEBA water model using GEM distributed multipoles. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	20
56	Structural and computational dissection of the catalytic mechanism of the inorganic pyrophosphatase from Mycobacterium tuberculosis. Journal of Structural Biology, 2015, 192, 76-87.	1.3	14
57	Computational Study of Putative Residues Involved in DNA Synthesis Fidelity Checking in Thermus aquaticus DNA Polymerase I. Advances in Protein Chemistry and Structural Biology, 2014, 96, 39-75.	1.0	12
58	Classical Electrostatics for Biomolecular Simulations. Chemical Reviews, 2014, 114, 779-814.	23.0	229
59	Homology modeling, molecular dynamics, and site-directed mutagenesis study of AlkB human homolog 1 (ALKBH1). Journal of Molecular Graphics and Modelling, 2014, 54, 123-130.	1.3	9
60	Alternative Pathway for the Reaction Catalyzed by DNA Dealkylase AlkB from Ab Initio QM/MM Calculations. Journal of Chemical Theory and Computation, 2014, 10, 5136-5148.	2.3	32
61	DFT-steric-based energy decomposition analysis of intermolecular interactions. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	43
62	GEM*: A Molecular Electronic Density-Based Force Field for Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 1361-1365.	2.3	64
63	S/G-1: An ab Initio Force-Field Blending Frozen Hermite Gaussian Densities and Distributed Multipoles. Proof of Concept and First Applications to Metal Cations. Journal of Physical Chemistry A, 2014, 118, 7598-7612.	1.1	22
64	Development of AMOEBA Force Field for 1,3-Dimethylimidazolium Based Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 7156-7166.	1.2	40
65	Disruption of Intrinsic Motions as a Mechanism for Enzyme Inhibition. Biophysical Journal, 2013, 105, 494-501.	0.2	2
66	Hypothesis driven single nucleotide polymorphism search (HyDn-SNP-S). DNA Repair, 2013, 12, 733-740.	1.3	11
67	Efficient optimization of van der Waals parameters from bulk properties. Journal of Computational Chemistry, 2013, 34, 2313-2319.	1.5	5
68	Exploring the structural determinants of selective phosphopeptide recognition using bivalent metal-coordination complexes. MedChemComm, 2013, 4, 289-292.	3.5	6
69	Electrostatics Interactions in Classical Simulations. Methods in Molecular Biology, 2013, 924, 243-270.	0.4	8
70	Toward a Deeper Understanding of Enzyme Reactions Using the Coupled ELF/NCI Analysis: Application to DNA Repair Enzymes. Journal of Chemical Theory and Computation, 2013, 9, 2156-2160.	2.3	48
71	Ab Initio QM/MM Calculations Show an Intersystem Crossing in the Hydrogen Abstraction Step in Dealkylation Catalyzed by AlkB. Journal of Physical Chemistry B, 2013, 117, 6410-6420.	1.2	58
72	Further refinements of next-generation force fields â€" Nonempirical localization of off-centered points in molecules. Canadian Journal of Chemistry, 2013, 91, 804-810.	0.6	10

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73	Novel Alkoxide Cluster Topologies Featuring Rare Seesaw Geometry at Transition Metal Centers. Chemistry - A European Journal, 2013, 19, 12225-12228.	1.7	31
74	Application of Gaussian Electrostatic Model (GEM) Distributed Multipoles in the AMOEBA Force Field. Journal of Chemical Theory and Computation, 2012, 8, 5072-5080.	2.3	57
75	Concentration-Independent pH Detection with a Luminescent Dimetallic Eu(III)-Based Probe. Journal of the American Chemical Society, 2012, 134, 17372-17375.	6.6	56
76	The Kinase Activity of the Helicobacter pylori Asp-tRNA^{Asn}/Glu-tRNA^{Gln} Amidotransferase Is Sensitive to Distal Mutations in Its Putative Ammonia Tunnel. Biochemistry, 2012, 51, 273-285.	1.2	6
77	Catalytic Mechanism of 4-Oxalocrotonate Tautomerase: Significances of Proteinâ€“Protein Interactions on Proton Transfer Pathways. Journal of Physical Chemistry B, 2012, 116, 6889-6897.	1.2	7
78	Computational Prediction of Residues Involved in Fidelity Checking for DNA Synthesis in DNA Polymerase I. Biochemistry, 2012, 51, 2569-2578.	1.2	29
79	Conformational Analysis of Clostridium difficile Toxin B and Its Implications for Substrate Recognition. PLoS ONE, 2012, 7, e41518.	1.1	3
80	Correlation between electron localization and metal ion mutagenicity in DNA synthesis from QM/MM calculations. Physical Chemistry Chemical Physics, 2011, 13, 11239.	1.3	18
81	Unraveling Lowâ€Barrier Hydrogen Bonds in Complex Systems with a Simple Quantum Topological Criterion. Chemistry - A European Journal, 2011, 17, 2833-2837.	1.7	11
82	DFT study of a model system for the dealkylation step catalyzed by AlkB. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 70-77.	2.2	14
83	Gaussian Multipole Model (GMM). Journal of Chemical Theory and Computation, 2010, 6, 190-202.	2.3	79
84	Reaction Mechanism of the Îµ Subunit of E. coli DNA Polymerase III: Insights into Active Site Metal Coordination and Catalytically Significant Residues. Journal of the American Chemical Society, 2009, 131, 1550-1556.	6.6	64
85	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
86	Simple formulas for improved pointâ€charge electrostatics in classical force fields and hybrid quantum mechanical/molecular mechanical embedding. International Journal of Quantum Chemistry, 2008, 108, 1905-1912.	1.0	53
87	Catalytic mechanism of human DNA polymerase Î» with Mg2+ and Mn2+ from ab initio quantum mechanical/molecular mechanical studies. DNA Repair, 2008, 7, 1824-1834.	1.3	52
88	Numerical Fitting of Molecular Properties to Hermite Gaussians. Journal of Physical Chemistry A, 2007, 111, 12049-12056.	1.1	36
89	Anisotropic, Polarizable Molecular Mechanics Studies of Inter- and Intramolecular Interactions and Ligandâ^'Macromolecule Complexes. A Bottom-Up Strategy. Journal of Chemical Theory and Computation, 2007, 3, 1960-1986.	2.3	312
90	Towards a force field based on density fitting. Journal of Chemical Physics, 2006, 124, 104101.	1.2	175

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91	Theoretical and Experimental Determination on Two Substrates Turned over by 4-Oxalocrotonate Tautomeraseâ€. Journal of Physical Chemistry A, 2006, 110, 700-708.	1.1	21
92	Quantum Mechanics/Molecular Mechanics Electrostatic Embedding with Continuous and Discrete Functions. Journal of Physical Chemistry B, 2006, 110, 13682-13684.	1.2	53
93	Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. Journal of Chemical Physics, 2006, 125, 054511.	1.2	169
94	Generalization of the Gaussian electrostatic model: Extension to arbitrary angular momentum, distributed multipoles, and speedup with reciprocal space methods. Journal of Chemical Physics, 2006, 125, 184101.	1.2	100
95	Reaction path determination for quantum mechanical/molecular mechanical modeling of enzyme reactions by combining first order and second order â€œchain-of-replicasâ€•methods. Journal of Chemical Physics, 2005, 122, 114502.	1.2	36
96	Intermolecular electrostatic energies using density fitting. Journal of Chemical Physics, 2005, 123, 044109.	1.2	55
97	Parallel iterative reaction path optimization in ab initio quantum mechanical/molecular mechanical modeling of enzyme reactions. Journal of Chemical Physics, 2004, 121, 697-706.	1.2	43
98	The Protein Backbone Makes Important Contributions to 4-Oxalocrotonate Tautomerase Enzyme Catalysis:Â Understanding from Theory and Experimentâ€. Biochemistry, 2004, 43, 6885-6892.	1.2	64
99	Dramatic effect of homoallylic substitution on the rate of palladium-catalyzed diene cycloisomerization. Journal of Organometallic Chemistry, 2003, 687, 498-507.	0.8	15
100	Ab Initio QM/MM Study Shows There Is No General Acid in the Reaction Catalyzed by 4-Oxalocrotonate Tautomerase. Journal of the American Chemical Society, 2003, 125, 10384-10393.	6.6	89
101	DFT study of the structural and electronic properties of small Nin (n=2-4) clusters. International Journal of Quantum Chemistry, 1999, 75, 847-861.	1.0	35