

Pedro E. M. Lopes

List of Publications by Year in descending order

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35
papers

10,907
citations

304743

22
h-index

395702

33
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36
all docs

36
docs citations

36
times ranked

14189
citing authors

#	ARTICLE	IF	CITATIONS
1	CHARMM general force field: A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields. <i>Journal of Computational Chemistry</i> , 2010, 31, 671-690.	3.3	4,718
2	Optimization of the Additive CHARMM All-Atom Protein Force Field Targeting Improved Sampling of the Backbone ϕ , ψ and Side-Chain χ_1 and χ_2 Dihedral Angles. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3257-3273.	5.3	3,696
3	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5430-5449.	5.3	329
4	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability: theory and applications. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 11-28.	1.4	314
5	Development of an Empirical Force Field for Silica. Application to the Quartz-Water Interface. <i>Journal of Physical Chemistry B</i> , 2006, 110, 2782-2792.	2.6	209
6	Recent developments and applications of the CHARMM force fields. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 167-185.	14.6	173
7	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9142-9160.	2.6	159
8	Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2873-2885.	2.6	149
9	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1587-1597.	5.3	142
10	Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3144-3150.	4.6	139
11	Current Status of Protein Force Fields for Molecular Dynamics Simulations. <i>Methods in Molecular Biology</i> , 2015, 1215, 47-71.	0.9	139
12	Accurate Calculation of Hydration Free Energies using Pair-Specific Lennard-Jones Parameters in the CHARMM Drude Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1181-1198.	5.3	131
13	Six-site polarizable model of water based on the classical Drude oscillator. <i>Journal of Chemical Physics</i> , 2013, 138, 034508.	3.0	103
14	Polarizable empirical force field for nitrogen-containing heteroaromatic compounds based on the classical Drude oscillator. <i>Journal of Computational Chemistry</i> , 2009, 30, 1821-1838.	3.3	65
15	The Small Molecule IMR-1 Inhibits the Notch Transcriptional Activation Complex to Suppress Tumorigenesis. <i>Cancer Research</i> , 2016, 76, 3593-3603.	0.9	60
16	Polarizable Empirical Force Field for Acyclic Polyalcohols Based on the Classical Drude Oscillator. <i>Biopolymers</i> , 2013, 99, 724-738.	2.4	50
17	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 993-1004.	5.4	45
18	Inhibition of the Bacterial Heme Oxygenases from <i>Pseudomonas aeruginosa</i> and <i>Neisseria meningitidis</i> : Novel Antimicrobial Targets. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 3804-3813.	6.4	38

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19	Holo-Ni(II)HpNikR Is an Asymmetric Tetramer Containing Two Different Nickel-Binding Sites. <i>Journal of the American Chemical Society</i> , 2010, 132, 14447-14456.	13.7	36
20	Kirkwood-Buff analysis of aqueous N-methylacetamide and acetamide solutions modeled by the CHARMM additive and Drude polarizable force fields. <i>Journal of Chemical Physics</i> , 2013, 139, 084509.	3.0	31
21	Small Molecule Antivirulents Targeting the Iron-Regulated Heme Oxygenase (HemO) of <i>P. aeruginosa</i> . <i>Journal of Medicinal Chemistry</i> , 2013, 56, 2097-2109.	6.4	27
22	An $\hat{\sigma}$ -atoms in molecules $\hat{\sigma}$ ™ (AIM) analysis of the dihydrogen bond in organometallic compounds. <i>Journal of Organometallic Chemistry</i> , 2000, 609, 53-59.	1.8	26
23	Intrinsic Energy Landscapes of Amino Acid Side-Chains. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1559-1572.	5.4	19
24	The effect of the counter ion on $M\hat{\sigma}^{\text{H}}\hat{\sigma}^{\text{A}}\hat{\sigma}^{\text{H}}\hat{\sigma}^{\text{X}}$ (X=O, N) interactions in crystalline transition metal hydrides. <i>New Journal of Chemistry</i> , 1999, 23, 219-226.	2.8	18
25	Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin Using a Combined Grand Canonical Monte Carlo/Molecular Dynamics Simulation Approach. <i>PLoS Computational Biology</i> , 2013, 9, e1003113.	3.2	18
26	Reconstruction of the (011) surface on $\hat{\sigma}$ quartz: A semiclassical <i>Ab initio</i> molecular dynamics study. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 50-64.	2.0	17
27	Organometallic Cluster Complexes with Face-Capping Arene Ligands. 8. Nucleophilic Reactivity of Cluster Complexes with Face-Capping Arene Ligands: $\hat{\sigma}$ Metal vs Ligand Protonation. <i>Organometallics</i> , 1996, 15, 5622-5634.	2.3	16
28	Molecular structure and crystal structure generation for $[Fe_3(CO)_{12}]$. <i>Journal of the Chemical Society Dalton Transactions</i> , 1995, , 3297.	1.1	12
29	Ferrocenylsilatranes a synthetic, structural and theoretical investigation. <i>Journal of Organometallic Chemistry</i> , 1997, 543, 93-102.	1.8	10
30	Formalisms for the Explicit Inclusion of Electronic Polarizability in Molecular Modeling and Dynamics Studies. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2009, , 219-257.	0.6	8
31	Development of the Charmm Polarizable Force Field for Polypeptides Based on Drude Oscillators. <i>Biophysical Journal</i> , 2011, 100, 612a.	0.5	5
32	Insertion of isonitrile into the $Mo\hat{\sigma}^{\text{C}}$ bond of $[MoCp_2(CH_3)(CNH)]^+$: a density functional study. <i>New Journal of Chemistry</i> , 2000, 24, 289-293.	2.8	3
33	Ion Channel Simulation with Explicit Solvent and Lipid Membrane Based on the Drude Polarizable Force Field. <i>Biophysical Journal</i> , 2014, 106, 44a.	0.5	1
34	Development of a Polarizable Force Field for Macromolecules Based on the Classical Drude Oscillator. <i>Biophysical Journal</i> , 2014, 106, 43a.	0.5	0
35	Fast calculation of two-electron-repulsion integrals: a numerical approach. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	0