Pedro E. M. Lopes

List of Publications by Year
in descending order

35	10,907	304743 22	395702 33
papers	citations	h-index	g-index

36	36	36	14189
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	5.4	45
2	Fast calculation of two-electron-repulsion integrals: a numerical approach. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	0
3	The Small Molecule IMR-1 Inhibits the Notch Transcriptional Activation Complex to Suppress Tumorigenesis. Cancer Research, 2016, 76, 3593-3603.	0.9	60
4	Current Status of Protein Force Fields for Molecular Dynamics Simulations. Methods in Molecular Biology, 2015, 1215, 47-71.	0.9	139
5	Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model. Journal of Physical Chemistry Letters, 2014, 5, 3144-3150.	4.6	139
6	Development of a Polarizable Force Field for Macromolecules Based on the Classical Drude Oscillator. Biophysical Journal, 2014, 106, 43a.	0.5	0
7	Ion Channel Simulation with Explicit Solvent and Lipid Membrane Based on the Drude Polarizable Force Field. Biophysical Journal, 2014, 106, 44a.	0.5	1
8	Polarizable Empirical Force Field for Acyclic Polyalcohols Based on the Classical Drude Oscillator. Biopolymers, 2013, 99, 724-738.	2.4	50
9	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2013, 9, 5430-5449.	5.3	329
10	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. Journal of Physical Chemistry B, 2013, 117, 9142-9160.	2.6	159
11	Kirkwood-Buff analysis of aqueous N-methylacetamide and acetamide solutions modeled by the CHARMM additive and Drude polarizable force fields. Journal of Chemical Physics, 2013, 139, 084509.	3.0	31
12	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	3.0	103
13	Small Molecule Antivirulents Targeting the Iron-Regulated Heme Oxygenase (HemO) of P. aeruginosa. Journal of Medicinal Chemistry, 2013, 56, 2097-2109.	6.4	27
14	Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin Using a Combined Grand Canonical Monte Carlo/Molecular Dynamics Simulation Approach. PLoS Computational Biology, 2013, 9, e1003113.	3.2	18
15	Intrinsic Energy Landscapes of Amino Acid Side-Chains. Journal of Chemical Information and Modeling, 2012, 52, 1559-1572.	5.4	19
16	Optimization of the Additive CHARMM All-Atom Protein Force Field Targeting Improved Sampling of the Backbone Ï•, Ï^ and Side-Chain Ï‡₁ and Ï‡₂ Dihedral Angles. Journal of Chemical Theory and Computation, 2012, 8, 3257-3273.	5.3	3,696
17	Recent developments and applications of the CHARMM force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 167-185.	14.6	173
18	Development of the Charmm Polarizable Force Field for Polypeptides Based on Drude Oscillators. Biophysical Journal, 2011, 100, 612a.	0.5	5

#	Article	IF	Citations
19	CHARMM general force field: A force field for drugâ€like molecules compatible with the CHARMM allâ€atom additive biological force fields. Journal of Computational Chemistry, 2010, 31, 671-690.	3.3	4,718
20	Holo-Ni(II)HpNikR Is an Asymmetric Tetramer Containing Two Different Nickel-Binding Sites. Journal of the American Chemical Society, 2010, 132, 14447-14456.	13.7	36
21	Accurate Calculation of Hydration Free Energies using Pair-Specific Lennard-Jones Parameters in the CHARMM Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 1181-1198.	5.3	131
22	Polarizable empirical force field for nitrogenâ€containing heteroaromatic compounds based on the classical Drude oscillator. Journal of Computational Chemistry, 2009, 30, 1821-1838.	3.3	65
23	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability: theory and applications. Theoretical Chemistry Accounts, 2009, 124, 11-28.	1.4	314
24	Reconstruction of the (011) surface on Î±â€quartz: A semiclassical Ab initio molecular dynamics study. International Journal of Quantum Chemistry, 2009, 109, 50-64.	2.0	17
25	Formalisms for the Explicit Inclusion of Electronic Polarizability in Molecular Modeling and Dynamics Studies. Challenges and Advances in Computational Chemistry and Physics, 2009, , 219-257.	0.6	8
26	Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2007, 111, 2873-2885.	2.6	149
27	Inhibition of the Bacterial Heme Oxygenases from Pseudomonas aeruginosa and Neisseria meningitidis:â€‰ Novel Antimicrobial Targets. Journal of Medicinal Chemistry, 2007, 50, 3804-3813.	6.4	38
28	Development of an Empirical Force Field for Silica. Application to the Quartzâ^'Water Interface. Journal of Physical Chemistry B, 2006, 110, 2782-2792.	2.6	209
29	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2006, 2, 1587-1597.	5.3	142
30	An â€˜atoms in moleculesâ€™ (AIM) analysis of the dihydrogen bond in organometallic compounds. Journal of Organometallic Chemistry, 2000, 609, 53-59.	1.8	26
31	Insertion of isonitrile into the Moâ€“C bond of [MoCp2(CH3)(CNH)]+: a density functional study. New Journal of Chemistry, 2000, 24, 289-293.	2.8	3
32	The effect of the counter ion on Mâ€“HÂ·Â·Â·Hâ€“X (X=O, N) interactions in crystalline transition metal hydrides. New Journal of Chemistry, 1999, 23, 219-226.	2.8	18
33	Ferrocenylsilatranes a synthetic, structural and theoretical investigation. Journal of Organometallic Chemistry, 1997, 543, 93-102.	1.8	10
34	Organometallic Cluster Complexes with Face-Capping Arene Ligands. 8. Nucleophilic Reactivity of Cluster Complexes with Face-Capping Arene Ligands:â€‰ Metal vs Ligand Protonation. Organometallics, 1996, 15, 5622-5634.	2.3	16
35	Molecular structure and crystal structure generation for [Fe3(CO)12]. Journal of the Chemical Society Dalton Transactions, 1995, , 3297.	1.1	12