Pedro E M Lopes

List of Publications by Year in descending order

20 papers	5,980 citations	394421 19 h-index	794594 19 g-index
20 all docs	20 docs citations	20 times ranked	8241 citing authors

#	Article	IF	Citations
1	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
2	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
3	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability: theory and applications. Theoretical Chemistry Accounts, 2009, 124, 11-28.	1.4	314
4	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
5	Recent developments and applications of the CHARMM force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 167-185.	14.6	173
6	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
7	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
8	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
9	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
10	Current Status of Protein Force Fields for Molecular Dynamics Simulations. Methods in Molecular Biology, 2015, 1215, 47-71.	0.9	139
11	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
12	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	3.0	103
13	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
14	The Small Molecule IMR-1 Inhibits the Notch Transcriptional Activation Complex to Suppress Tumorigenesis. Cancer Research, 2016, 76, 3593-3603.	0.9	60
15	Polarizable Empirical Force Field for Acyclic Polyalcohols Based on the Classical Drude Oscillator. Biopolymers, 2013, 99, 724-738.	2.4	50
16	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
17	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
18	Small Molecule Antivirulents Targeting the Iron-Regulated Heme Oxygenase (HemO) of P. aeruginosa. Journal of Medicinal Chemistry, 2013, 56, 2097-2109.	6.4	27

#	Article	IF	Citations
19	Intrinsic Energy Landscapes of Amino Acid Side-Chains. Journal of Chemical Information and Modeling, 2012, 52, 1559-1572.	5.4	19
20	Fast calculation of two-electron-repulsion integrals: a numerical approach. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	0