Anmol Kumar

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4641501/publications.pdf

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20 papers	490 citations	840776 11 h-index	839539 18 g-index
20 all docs	20 docs citations	20 times ranked	536 citing authors

#	Article	IF	Citations
1	Deep Neural Network Model to Predict the Electrostatic Parameters in the Polarizable Classical Drude Oscillator Force Field. Journal of Chemical Theory and Computation, 2022, 18, 1711-1725.	5.3	13
2	Harnessing Deep Learning for Optimization of Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field. Journal of Chemical Theory and Computation, 2022, 18, 2388-2407.	5.3	17
3	Luminescent naphthalimide-tagged ruthenium(<scp>ii</scp>)â€“arene complexes: cellular imaging, photocytotoxicity and transferrin binding. Dalton Transactions, 2021, 50, 3629-3640.	3.3	12
4	Stereoisomerization of human constitutive androstane receptor agonist CITCO. Tetrahedron, 2021, 79, 131886.	1.9	1
5	Additive CHARMM36 Force Field for Nonstandard Amino Acids. Journal of Chemical Theory and Computation, 2021, 17, 3554-3570.	5.3	39
6	Inhibition Ability of Natural Compounds on Receptor-Binding Domain of SARS-CoV2: An In Silico Approach. Pharmaceuticals, 2021, 14, 1328.	3.8	10
7	FFParam: Standalone package for CHARMM additive and Drude polarizable force field parametrization of small molecules. Journal of Computational Chemistry, 2020, 41, 958-970.	3.3	50
8	Predicting Partition Coefficients of Neutral and Charged Solutes in the Mixed SLESâ€“Fatty Acid Micellar System. Journal of Physical Chemistry B, 2020, 124, 1653-1664.	2.6	5
9	Use of Cyano Probes in QM/MM Simulations to Study the Effect of Ion Concentration and Temperature of the Environment on a Uracil Nucleotide and DNA. Biophysical Journal, 2019, 116, 357a.	0.5	0
10	Topology of molecular electron density and electrostatic potential with DAMQT. Computer Physics Communications, 2017, 214, 207-215.	7.5	25
11	Molecular Electrostatic Potential-Based Atoms in Molecules: Shielding Effects and Reactivity Patterns. Australian Journal of Chemistry, 2016, 69, 975.	0.9	7
12	Bonding and Reactivity Patterns from Electrostatic Landscapes of Molecules. Journal of Chemical Sciences, 2016, 128, 1519-1526.	1.5	9
13	Exploring the Gradient Paths and Zero Flux Surfaces of Molecular Electrostatic Potential. Journal of Chemical Theory and Computation, 2016, 12, 1705-1713.	5.3	17
14	DAMQT 2.1.0: A new version of the DAMQT package enabled with the topographical analysis of electron density and electrostatic potential in molecules. Journal of Computational Chemistry, 2015, 36, 2350-2359.	3.3	47
15	Understanding Lone Pair-Ï€ Interactions from Electrostatic Viewpoint. Challenges and Advances in Computational Chemistry and Physics, 2015, , 391-418.	0.6	9
16	Hybrid QTAIM and electrostatic potential-based quantum topology phase diagrams for water clusters. Physical Chemistry Chemical Physics, 2015, 17, 15258-15273.	2.8	9
17	On the electrostatic nature of electrides. Physical Chemistry Chemical Physics, 2015, 17, 15030-15035.	2.8	15
18	Lone Pairs: An Electrostatic Viewpoint. Journal of Physical Chemistry A, 2014, 118, 526-532.	2.5	89

#	Article	IF	Citations
19	Stabilization of Si(0) and Ge(0) compounds by different silylenes and germylenes: a density functional and molecular electrostatic study. Dalton Transactions, 2013, 42, 13200.	3.3	22
20	Molecular electrostatics for probing lone pairâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2013, 15, 18401.	2.8	94