

# Anmol Kumar

## List of Publications by Year in descending order

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Version: 2024-02-01

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	Molecular electrostatics for probing lone pair interactions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18401.	2.8	94
2	Lone Pairs: An Electrostatic Viewpoint. <i>Journal of Physical Chemistry A</i> , 2014, 118, 526-532.	2.5	89
3	FFParam: Standalone package for CHARMM additive and Drude polarizable force field parametrization of small molecules. <i>Journal of Computational Chemistry</i> , 2020, 41, 958-970.	3.3	50
4	DAMQT 2.1.0: A new version of the DAMQT package enabled with the topographical analysis of electron density and electrostatic potential in molecules. <i>Journal of Computational Chemistry</i> , 2015, 36, 2350-2359.	3.3	47
5	Additive CHARMM36 Force Field for Nonstandard Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3554-3570.	5.3	39
6	Topology of molecular electron density and electrostatic potential with DAMQT. <i>Computer Physics Communications</i> , 2017, 214, 207-215.	7.5	25
7	Stabilization of Si(0) and Ge(0) compounds by different silylenes and germlyenes: a density functional and molecular electrostatic study. <i>Dalton Transactions</i> , 2013, 42, 13200.	3.3	22
8	Exploring the Gradient Paths and Zero Flux Surfaces of Molecular Electrostatic Potential. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1705-1713.	5.3	17
9	Harnessing Deep Learning for Optimization of Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2388-2407.	5.3	17
10	On the electrostatic nature of electrides. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15030-15035.	2.8	15
11	Deep Neural Network Model to Predict the Electrostatic Parameters in the Polarizable Classical Drude Oscillator Force Field. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1711-1725.	5.3	13
12	Luminescent naphthalimide-tagged ruthenium(II) arene complexes: cellular imaging, photocytotoxicity and transferrin binding. <i>Dalton Transactions</i> , 2021, 50, 3629-3640.	3.3	12
13	Inhibition Ability of Natural Compounds on Receptor-Binding Domain of SARS-CoV2: An In Silico Approach. <i>Pharmaceuticals</i> , 2021, 14, 1328.	3.8	10
14	Understanding Lone Pair Interactions from Electrostatic Viewpoint. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 391-418.	0.6	9
15	Hybrid QTAIM and electrostatic potential-based quantum topology phase diagrams for water clusters. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15258-15273.	2.8	9
16	Bonding and Reactivity Patterns from Electrostatic Landscapes of Molecules. <i>Journal of Chemical Sciences</i> , 2016, 128, 1519-1526.	1.5	9
17	Molecular Electrostatic Potential-Based Atoms in Molecules: Shielding Effects and Reactivity Patterns. <i>Australian Journal of Chemistry</i> , 2016, 69, 975.	0.9	7
18	Predicting Partition Coefficients of Neutral and Charged Solutes in the Mixed SLES Fatty Acid Micellar System. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1653-1664.	2.6	5

#	ARTICLE	IF	CITATIONS
19	Stereoisomerization of human constitutive androstane receptor agonist CITCO. Tetrahedron, 2021, 79, 131886.	1.9	1
20	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