

David M Rogers

List of Publications by Year in descending order

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28
papers

1,610
citations

567281

15
h-index

526287

27
g-index

29
all docs

29
docs citations

29
times ranked

2848
citing authors

#	ARTICLE	IF	CITATIONS
1	Very fast prediction and rationalization of pK_a values for protein-ligand complexes. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 765-783.	2.6	938
2	Electronic Circular Dichroism Spectroscopy of Proteins. <i>CheM</i> , 2019, 5, 2751-2774.	11.7	100
3	Can Dispersion Forces Govern Aromatic Stacking in an Organic Solvent?. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 912-916.	13.8	82
4	First-Principles Calculations of Protein Circular Dichroism in the Near Ultraviolet. <i>Biochemistry</i> , 2004, 43, 11092-11102.	2.5	71
5	Ab Initio Study of Aromatic Side Chains of Amino Acids in Gas Phase and Solution. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11191-11200.	2.5	48
6	Modeling the Absorption Spectrum of Tryptophan in Proteins. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23061-23069.	2.6	46
7	Quantifying signal changes in nano-wire based biosensors. <i>Nanoscale</i> , 2011, 3, 706-717.	5.6	37
8	How focussing on hydrogen bonding interactions in amino acids can miss the bigger picture: a high-pressure neutron powder diffraction study of β -glycine. <i>CrystEngComm</i> , 2015, 17, 5315-5328.	2.6	35
9	Can Dispersion Forces Govern Aromatic Stacking in an Organic Solvent?. <i>Angewandte Chemie</i> , 2016, 128, 924-928.	2.0	28
10	Calculations of protein circular dichroism from first principles. <i>Chirality</i> , 2004, 16, 234-243.	2.6	27
11	Ab initio study of the toluene dimer. <i>Chemical Physics Letters</i> , 2006, 427, 410-413.	2.6	25
12	Catalytic Role of the Substrate Defines Specificity of Therapeutic L-Asparaginase. <i>Journal of Molecular Biology</i> , 2015, 427, 2867-2885.	4.2	25
13	Functionalised metal-organic frameworks: a novel approach to stabilising single metal atoms. <i>Journal of Materials Chemistry A</i> , 2017, 5, 15559-15566.	10.3	24
14	Femtosecond photodissociation dynamics of 1,4-diiodobenzene by gas-phase X-ray scattering and photoelectron spectroscopy. <i>Faraday Discussions</i> , 2016, 194, 525-536.	3.2	23
15	Coherent ultrafast lattice-directed reaction dynamics of triiodide anion photodissociation. <i>Nature Chemistry</i> , 2017, 9, 516-522.	13.6	16
16	Dewar Benzenoids Discovered In Carbon Nanobelts. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3769-3772.	4.6	13
17	Metal-to-metal charge-transfer transitions in Prussian blue hexacyanochromate analogues. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2018, 227, 28-38.	3.5	11
18	CASSCF study of energies and lifetimes of temporary negative ions of CH_2Br_2 , CHClBr_2 and CCl_3Br . <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 447-451.	2.8	10

#	ARTICLE	IF	CITATIONS
19	Preorganized tridentate analogues of mixed hydroxyoxime/carboxylate nickel extractants. Dalton Transactions, 2016, 45, 3734-3742.	3.3	9
20	Force Fields for Macromolecular Assemblies Containing Diketopyrrolopyrrole and Thiophene. Journal of Chemical Theory and Computation, 2020, 16, 5150-5162.	5.3	9
21	On the choice of active space orbitals in MCSCF calculations. Computational and Theoretical Chemistry, 1998, 434, 239-245.	1.5	8
22	A theoretical and experimental study of the HPCI radical: the $\hat{\pi}^* \leftarrow \pi$ visible emission spectrum. Chemical Physics Letters, 2000, 331, 483-488.	2.6	8
23	Salicylaldehyde Hydrazones: Buttressing of Outer-Sphere Hydrogen-Bonding and Copper Extraction Properties. Australian Journal of Chemistry, 2017, 70, 556.	0.9	5
24	Ultrafast photodissociation dynamics of 1,4-diiodobenzene. Journal of Chemical Physics, 2018, 148, 194306.	3.0	5
25	A combined resonance enhanced multiphoton ionization and ab initio study of the first absorption band of 1,2,4,5-tetrafluorobenzene, pentafluorobenzene, and hexafluorobenzene. Journal of Chemical Physics, 2014, 141, 154310.	3.0	4
26	Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides. Molecules, 2021, 26, 396.	3.8	2
27	An efficient string-based truncation scheme for MCSCF calculations. Computational and Theoretical Chemistry, 1998, 452, 49-54.	1.5	1
28	Towards Atomically-Resolved Structural Changes during a Solid State Geminate Recombination Reaction. , 2016, , .		0