David M Rogers

List of Publications by Year
in descending order

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	Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides. Molecules, 2021, 26, 396.	3.8	2
2	Force Fields for Macromolecular Assemblies Containing Diketopyrrolopyrrole and Thiophene. Journal of Chemical Theory and Computation, 2020, 16, 5150-5162.	5.3	9
3	Dewar Benzenoids Discovered In Carbon Nanobelts. Journal of Physical Chemistry Letters, 2020, 11, 3769-3772.	4.6	13
4	Electronic Circular Dichroism Spectroscopy of Proteins. CheM, 2019, 5, 2751-2774.	11.7	100
5	Metal-to-metal charge-transfer transitions in Prussian blue hexacyanochromate analogues. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2018, 227, 28-38.	3.5	11
6	Ultrafast photodissociation dynamics of 1,4-diiodobenzene. Journal of Chemical Physics, 2018, 148, 194306.	3.0	5
7	Salicylaldehyde Hydrazones: Buttressing of Outer-Sphere Hydrogen-Bonding and Copper Extraction Properties. Australian Journal of Chemistry, 2017, 70, 556.	0.9	5
8	Functionalised metalâ€“organic frameworks: a novel approach to stabilising single metal atoms. Journal of Materials Chemistry A, 2017, 5, 15559-15566.	10.3	24
9	Coherent ultrafast lattice-directed reaction dynamics of triiodide anion photodissociation. Nature Chemistry, 2017, 9, 516-522.	13.6	16
10	Can Dispersion Forces Govern Aromatic Stacking in an Organic Solvent?. Angewandte Chemie - International Edition, 2016, 55, 912-916.	13.8	82
11	Femtosecond photodissociation dynamics of 1,4-diiodobenzene by gas-phase X-ray scattering and photoelectron spectroscopy. Faraday Discussions, 2016, 194, 525-536.	3.2	23
12	Can Dispersion Forces Govern Aromatic Stacking in an Organic Solvent?. Angewandte Chemie, 2016, 128, 924-928.	2.0	28
13	Preorganized tridentate analogues of mixed hydroxyoxime/carboxylate nickel extractants. Dalton Transactions, 2016, 45, 3734-3742.	3.3	9
14	Towards Atomically-Resolved Structural Changes during a Solid State Geminate Recombination Reaction. , 2016, , .		0
15	How focussing on hydrogen bonding interactions in amino acids can miss the bigger picture: a high-pressure neutron powder diffraction study of Îµ-glycine. CrystEngComm, 2015, 17, 5315-5328.	2.6	35
16	Catalytic Role of the Substrate Defines Specificity of Therapeutic l-Asparaginase. Journal of Molecular Biology, 2015, 427, 2867-2885.	4.2	25
17	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
18	Quantifying signal changes in nano-wire based biosensors. Nanoscale, 2011, 3, 706-717.	5.6	37

#	Article	IF	Citations
19	Very fast prediction and rationalization of pK_a values for proteinâ€“ligand complexes. Proteins: Structure, Function and Bioinformatics, 2008, 73, 765-783.	2.6	938
20	Ab initio study of the toluene dimer. Chemical Physics Letters, 2006, 427, 410-413.	2.6	25
21	Modeling the Absorption Spectrum of Tryptophan in Proteins. Journal of Physical Chemistry B, 2005, 109, 23061-23069.	2.6	46
22	Calculations of protein circular dichroism from first principles. Chirality, 2004, 16, 234-243.	2.6	27
23	First-Principles Calculations of Protein Circular Dichroism in the Near Ultravioletâ€. Biochemistry, 2004, 43, 11092-11102.	2.5	71
24	Ab Initio Study of Aromatic Side Chains of Amino Acids in Gas Phase and Solution. Journal of Physical Chemistry A, 2003, 107, 11191-11200.	2.5	48
25	A theoretical and experimental study of the HPCl radical: the â†'â€³ visible emission spectrum. Chemical Physics Letters, 2000, 331, 483-488.	2.6	8
26	CASSCF study of energies and lifetimes of temporary negative ions of CH2Br2, CHClBr2 and CCl3Br. Physical Chemistry Chemical Physics, 2000, 2, 447-451.	2.8	10
27	An efficient string-based truncation scheme for MCSCF calculations. Computational and Theoretical Chemistry, 1998, 452, 49-54.	1.5	1
28	On the choice of active space orbitals in MCSCF calculations. Computational and Theoretical Chemistry, 1998, 434, 239-245.	1.5	8