Damian G Allis

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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ext. citations4.8
avg, IF2.98
L-index

#	Paper	IF	Citations
16	Theoretical analysis of the terahertz spectrum of the high explosive PETN. <i>ChemPhysChem</i> , 2006 , 7, 23	898 .4 08	8 86
15	Importance of Vibrational Zero-Point Energy Contribution to the Relative Polymorph Energies of Hydrogen-Bonded Species. <i>Crystal Growth and Design</i> , 2008 , 8, 3905-3907	3.5	41
14	The inelastic neutron scattering spectrum of H3B:NH3 and the reproduction of its solid-state features by periodic DFT. <i>Journal of the American Chemical Society</i> , 2004 , 126, 7756-7	16.4	38
13	Experimental and theoretical studies of tetramethoxy-p-benzoquinone: infrared spectra, structural and lithium insertion properties. <i>RSC Advances</i> , 2013 , 3, 19081	3.7	20
12	Inelastic neutron scattering spectrum of Cs2[B12H12]: reproduction of its solid-state vibrational spectrum by periodic DFT. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 3744-9	2.8	18
11	Density Functional Dependence in the Theoretical Analysis of the Terahertz Spectrum of the Illicit Drug MDMA (Ecstasy). <i>IEEE Sensors Journal</i> , 2010 , 10, 478-484	4	16
10	The binding of vitamin B12 to transcobalamin(II); structural considerations for bioconjugate designa molecular dynamics study. <i>Molecular BioSystems</i> , 2010 , 6, 1611-8		14
9	Examining the effects of vitamin B12 conjugation on the biological activity of insulin: a molecular dynamic and in vivo oral uptake investigation. <i>MedChemComm</i> , 2012 , 3, 1054	5	11
8	Evaluating the friction of rotary joints in molecular machines. <i>Molecular Systems Design and Engineering</i> , 2017 , 2, 235-252	4.6	7
7	Commensurate Urea Inclusion Crystals with the Guest (E,E)-1,4-Diiodo-1,3-Butadiene. <i>Crystal Growth and Design</i> , 2013 , 13, 3852-3855	3.5	7
6	The low/room-temperature forms of the lithiated salt of 3,6-dihydroxy-2,5-dimethoxy-p-benzoquinone: a combined experimental and dispersion-corrected density functional study. <i>CrystEngComm</i> , 2013 , 15, 2809	3.3	7
5	Solution Structure and Constrained Molecular Dynamics Study of Vitamin B12 Conjugates of the Anorectic Peptide PYY(3-36). <i>ChemMedChem</i> , 2016 , 11, 1015-21	3.7	6
4	DEVELOPMENT OF COMPUTATIONAL METHODOLOGIES FOR THE PREDICTION AND ANALYSIS OF SOLID-STATE TERAHERTZ SPECTRA. <i>International Journal of High Speed Electronics and Systems</i> , 2007 , 17, 193-212	0.5	3
3	Preparation of Ordered Polyacetylene by Solid-State Polymerization in Nanoscale Confinement. <i>Chemistry of Materials</i> , 2020 , 32, 1769-1783	9.6	2
2	Insulated Polyacetylene Chains in an Inclusion Complex by Photopolymerization. <i>Materials Research Society Symposia Proceedings</i> , 2015 , 1799, 7-12		2
1	DEVELOPMENT OF COMPUTATIONAL METHODOLOGIES FOR THE PREDICTION AND ANALYSIS OF SOLID-STATE TERAHERTZ SPECTRA. <i>Selected Topics in Electornics and Systems</i> , 2007 , 1-20	О	