Damian G Allis

List of Publications by Year in Descending Order

16 papers	278 citations	8 h-index	16 g-index
18 ext. papers	297 ext. citations	4.8 avg, IF	2.98 L-index

#	Paper	IF	Citations
16	Preparation of Ordered Polyacetylene by Solid-State Polymerization in Nanoscale Confinement. *Chemistry of Materials*, **2020**, 32, 1769-1783	9.6	2
15	Evaluating the friction of rotary joints in molecular machines. *Molecular Systems Design and Engineering*, **2017**, 2, 235-252	4.6	7
14	Solution Structure and Constrained Molecular Dynamics Study of Vitamin B12 Conjugates of the Anorectic Peptide PYY(3-36). *ChemMedChem*, **2016**, 11, 1015-21	3.7	6
13	Insulated Polyacetylene Chains in an Inclusion Complex by Photopolymerization. *Materials Research Society Symposia Proceedings*, **2015**, 1799, 7-12		2
12	Commensurate Urea Inclusion Crystals with the Guest (E,E)-1,4-Diiodo-1,3-Butadiene. *Crystal Growth and Design*, **2013**, 13, 3852-3855	3.5	7
11	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. *CrystEngComm*, **2013**, 15, 2809	3.3	7
10	Experimental and theoretical studies of tetramethoxy-p-benzoquinone: infrared spectra, structural and lithium insertion properties. *RSC Advances*, **2013**, 3, 19081	3.7	20
9	Examining the effects of vitamin B12 conjugation on the biological activity of insulin: a molecular dynamic and in vivo oral uptake investigation. *MedChemComm*, **2012**, 3, 1054	5	11
8	The binding of vitamin B12 to transcobalamin(II); structural considerations for bioconjugate design--a molecular dynamics study. *Molecular BioSystems*, **2010**, 6, 1611-8		14
7	Density Functional Dependence in the Theoretical Analysis of the Terahertz Spectrum of the Illicit Drug MDMA (Ecstasy). *IEEE Sensors Journal*, **2010**, 10, 478-484	4	16
6	Importance of Vibrational Zero-Point Energy Contribution to the Relative Polymorph Energies of Hydrogen-Bonded Species. *Crystal Growth and Design*, **2008**, 8, 3905-3907	3.5	41
5	DEVELOPMENT OF COMPUTATIONAL METHODOLOGIES FOR THE PREDICTION AND ANALYSIS OF SOLID-STATE TERAHERTZ SPECTRA. *International Journal of High Speed Electronics and Systems*, **2007**, 17, 193-212	0.5	3
4	DEVELOPMENT OF COMPUTATIONAL METHODOLOGIES FOR THE PREDICTION AND ANALYSIS OF SOLID-STATE TERAHERTZ SPECTRA. *Selected Topics in Electornics and Systems*, **2007**, 1-20	0	
3	Theoretical analysis of the terahertz spectrum of the high explosive PETN. *ChemPhysChem*, **2006**, 7, 2398-408	3.2	86
2	Inelastic neutron scattering spectrum of Cs2[B12H12]: reproduction of its solid-state vibrational spectrum by periodic DFT. *Journal of Physical Chemistry A*, **2006**, 110, 3744-9	2.8	18
1	The inelastic neutron scattering spectrum of H3B:NH3 and the reproduction of its solid-state features by periodic DFT. *Journal of the American Chemical Society*, **2004**, 126, 7756-7	16.4	38