

Damian G Allis

List of Publications by Year in descending order

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18
all docs

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docs citations

18
times ranked

471
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical Analysis of the Terahertz Spectrum of the High Explosive PETN. <i>ChemPhysChem</i> , 2006, 7, 2398-2408.	2.1	98
2	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.	3.0	48
3	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, 7756-7757.	13.7	40
4	Experimental and theoretical studies of tetramethoxy-p-benzoquinone: infrared spectra, structural and lithium insertion properties. <i>RSC Advances</i> , 2013, 3, 19081.	3.6	21
5	Inelastic Neutron Scattering Spectrum of Cs2[B12H12]:Â Reproduction of Its Solid-State Vibrational Spectrum by Periodic DFT. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3744-3749.	2.5	19
6	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.	4.7	18
7	The binding of vitamin B12 to transcobalamin(II); structural considerations for bioconjugate designâ€”a molecular dynamics study. <i>Molecular BioSystems</i> , 2010, 6, 1611.	2.9	15
8	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.	3.4	11
9	Commensurate Urea Inclusion Crystals with the Guest (<i>E,E</i>)-1,4-Diiodo-1,3-Butadiene. <i>Crystal Growth and Design</i> , 2013, 13, 3852-3855.	3.0	9
10	Evaluating the friction of rotary joints in molecular machines. <i>Molecular Systems Design and Engineering</i> , 2017, 2, 235-252.	3.4	9
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. <i>CrystEngComm</i> , 2013, 15, 2809.	2.6	8
12	Preparation of Ordered Polyacetylene by Solid-State Polymerization in Nanoscale Confinement. <i>Chemistry of Materials</i> , 2020, 32, 1769-1783.	6.7	8
13	Solution Structure and Constrained Molecular Dynamics Study of Vitamin B₁₂ Conjugates of the Anorectic Peptide PYY(3â€“36). <i>ChemMedChem</i> , 2016, 11, 1015-1021.	3.2	6
14	Insulated Polyacetylene Chains in an Inclusion Complex by Photopolymerization. <i>Materials Research Society Symposia Proceedings</i> , 2015, 1799, 7-12.	0.1	4
15	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.	0.7	3
16	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.	0.2	0
17	Acyclic Identification of Aptamer from Over-Represented Libraries Using Hash Functions. , 2013, , .		0
18	A fast sorting algorithm for aptamer identification using deep sequencing. , 2014, , .		0