Angus Gray-Weale

List of Publications by Year
in descending order

64 papers	4,835 citations	159358 30 h-index	102304 66 g-index
70 all docs	70 docs citations	70 times ranked	7047 citing authors

#	Article	IF	Citations
1	Towards predicting the power conversion efficiencies of organic solar cells from donor and acceptor molecule structures. Journal of Materials Chemistry C, 2018, 6, 3276-3287.	2.7	17
2	Molecular Origin of Donor- and Acceptor-Rich Domain Formation in Bulk-Heterojunction Solar Cells with an Enhanced Charge Transport Efficiency. Journal of Physical Chemistry C, 2017, 121, 5864-5870.	1.5	18
3	Numerical analysis of a hysteresis model in perovskite solar cells. Computational Materials Science, 2017, 126, 22-28.	1.4	13
4	Hydrodynamic Drag on Diffusing Nanoparticles for Size Determination. Journal of Physical Chemistry C, 2016, 120, 21888-21896.	1.5	7
5	The coalescence of polystyrene in correlated binary solvents. Journal of Polymer Science, Part B: Polymer Physics, 2016, 54, 948-955.	2.4	3
6	A numerical model for charge transport and energy conversion of perovskite solar cells. Physical Chemistry Chemical Physics, 2016, 18, 4476-4486.	1.3	56
7	Pair correlations that link the hydrophobic and Hofmeister effects. Physical Chemistry Chemical Physics, 2016, 18, 14949-14959.	1.3	5
8	Liver glycogen in type 2 diabetic mice is randomly branched as enlarged aggregates with blunted glucose release. Glycoconjugate Journal, 2016, 33, 41-51.	1.4	15
9	From atomic structure to excess entropy: a neutron diffraction and density functional theory study of CaOâ”Al₂O₃â”SiO₂melts. Journal of Physics Condensed Matter, 2016, 28, 135102.	0.7	9
10	The biological function of an insect antifreeze protein simulated by molecular dynamics. ELife, 2015, 4, .	2.8	85
11	Photovoltaic performance and the energy landscape of CH₃NH₃PbI₃. Physical Chemistry Chemical Physics, 2015, 17, 22604-22615.	1.3	35
12	Modeling of Feâ€“W phase diagram using first principles and phonons calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 50, 92-104.	0.7	32
13	Ion-to-Neutral Ratios and Thermal Proton Transfer in Matrix-Assisted Laser Desorption/Ionization. Journal of the American Society for Mass Spectrometry, 2015, 26, 1242-1251.	1.2	36
14	Comment to the Reply on: â€œEnergetics and Kinetics of Thermal Ionization Models of MALDIâ€•by Richard Knochenmuss. J. Am. Soc. Mass Spectrom. 25, 1521â€“1527 (2014). Journal of the American Society for Mass Spectrometry, 2015, 26, 2169-2170.	1.2	2
15	Comment on: â€œEnergetics and Kinetics of Thermal Ionization Models of MALDIâ€•by Richard Knochenmuss. J. Am. Soc. Mass Spectrom. 25, 1521â€“1527 (2014). Journal of the American Society for Mass Spectrometry, 2015, 26, 2162-2166.	1.2	7
16	Order and correlation contributions to the entropy of hydrophobic solvation. Journal of Chemical Physics, 2015, 142, 114117.	1.2	17
17	Theoretical investigation on two-dimensional non-traditional carbon materials employing three-membered ring and four-membered ring as building blocks. Carbon, 2015, 95, 1033-1038.	5.4	22
18	pH and the surface tension of water. Journal of Colloid and Interface Science, 2014, 422, 54-57.	5.0	89

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19	Solubility of Sodium in Sodium Chloride: A Density Functional Theory Molecular Dynamics Study. Journal of the Electrochemical Society, 2014, 161, E3042-E3048.	1.3	15
20	A Fast Depositionâ€Crystallization Procedure for Highly Efficient Lead Iodide Perovskite Thinâ€Film Solar Cells. Angewandte Chemie - International Edition, 2014, 53, 9898-9903.	7.2	1,292
21	Gas-assisted preparation of lead iodide perovskite films consisting of a monolayer of single crystalline grains for high efficiency planar solar cells. Nano Energy, 2014, 10, 10-18.	8.2	504
22	Oil/Water Interface Charged by Hydroxide Ions and Deprotonated Fatty Acids: A Comment. Angewandte Chemie - International Edition, 2012, 51, 12941-12942.	7.2	40
23	Thermodynamic Limit of Exciton Fission Solar Cell Efficiency. Journal of Physical Chemistry Letters, 2012, 3, 2749-2754.	2.1	95
24	The structure of cardiac glycogen in healthy mice. International Journal of Biological Macromolecules, 2012, 51, 887-891.	3.6	36
25	The Surface Relaxation of Water. Journal of Physical Chemistry B, 2012, 116, 8981-8988.	1.2	26
26	Microenvironment-switchable singlet oxygen generation by axially-coordinated hydrophilic ruthenium phthalocyanine dendrimers. Physical Chemistry Chemical Physics, 2011, 13, 3385-3393.	1.3	19
27	Molecular Structural Differences between Type-2-Diabetic and Healthy Glycogen. Biomacromolecules, 2011, 12, 1983-1986.	2.6	43
28	Sodium Fluoride at the Air/Water Interface. Australian Journal of Chemistry, 2011, 64, 1580.	0.5	2
29	Hyperbranched alternating block copolymers using thiolâ€“yne chemistry: materials with tuneable properties. Chemical Communications, 2011, 47, 239-241.	2.2	100
30	Luminescent Hyperbranched Polymers: Combining Thiol-Yne Chemistry with Gold-Mediated Câ^'H Bond Activation. Organometallics, 2011, 30, 1315-1318.	1.1	47
31	Modeling highly branched structures: Description of the solution structures of dendrimers, polyglycerol, and glycogen. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 1525-1538.	2.4	7
32	Describing the Structure of a Randomly Hyperbranched Polymer. Macromolecular Theory and Simulations, 2010, 19, 219-227.	0.6	17
33	The structure of randomly branched polymers synthesized by living radical methods. Polymer Chemistry, 2010, 1, 1067.	1.9	33
34	Ab Initio Study of Water Polarization in the Hydration Shell of Aqueous Hydroxide: Comparison between Polarizable and Nonpolarizable Water Models. Journal of Chemical Theory and Computation, 2010, 6, 2888-2895.	2.3	16
35	Reply to the â€˜Comment on â€œAn explanation for the charge on water's surfaceâ€â€™ by R. VÃ¡cha, D. Horinek, R. Buchner, B. Winter and P. Jungwirth, Phys. Chem. Chem. Phys., 2010, 12, DOI: 10.1039/c001492c. Physical Chemistry Chemical Physics, 2010, 12, 14364.	1.3	9
36	A divergent synthesis of modular dendrimers via sequential Câ€“C bond fragmentation thio-Michael addition. Chemical Communications, 2010, 46, 6789.	2.2	10

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37	Nature of Î± and Î² Particles in Glycogen Using Molecular Size Distributions. Biomacromolecules, 2010, 11, 1094-1100.	2.6	72
38	RAFT polymerization kinetics: How long are the crossâ€terminating oligomers?. Journal of Polymer Science Part A, 2009, 47, 3455-3466.	2.5	82
39	General description of the structure of branched polymers. Journal of Polymer Science Part A, 2009, 47, 3914-3930.	2.5	35
40	Comment on â€˜Behaviour of hydroxide at the water/vapor interfaceâ€™ [Chem. Phys. Lett. 474 (2009) 241]. Chemical Physics Letters, 2009, 481, 22-24.	1.2	14
41	Correlations in the Structure and Dynamics of Ionic Liquids. Australian Journal of Chemistry, 2009, 62, 288.	0.5	9
42	Obtaining Kinetic Information from the Chain-Length Distribution of Polymers Produced by RAFT. Journal of Physical Chemistry B, 2009, 113, 7086-7094.	1.2	48
43	Comparative structural analyses of purified glycogen particles from rat liver, human skeletal muscle and commercial preparations. International Journal of Biological Macromolecules, 2009, 45, 478-482.	3.6	82
44	Searching for Stars: Selective Desulfurization and Fluorescence Spectroscopy as New Tools in the Search for Cross Termination Side-products in RAFT Polymerization. Australian Journal of Chemistry, 2009, 62, 1533.	0.5	19
45	Hyperbranched Polymers by Thiolâ€“Yne Chemistry: From Small Molecules to Functional Polymers. Journal of the American Chemical Society, 2009, 131, 18075-18077.	6.6	280
46	Extracting Physically Useful Information from Multiple-Detection Size-Separation Data for Starch. Biomacromolecules, 2009, 10, 2708-2713.	2.6	13
47	An explanation for the charge on waterâ€™s surface. Physical Chemistry Chemical Physics, 2009, 11, 10994.	1.3	145
48	RAFT Polymerization Kinetics: Combination of Apparently Conflicting Models. Macromolecules, 2008, 41, 6400-6412.	2.2	116
49	Statistical mechanical theory for steady state systems. VIII. General theory for a Brownian particle driven by a time- and space-varying force. Journal of Chemical Physics, 2008, 128, 114509.	1.2	7
50	Models for randomly hyperbranched polymers: Theory and simulation. Journal of Chemical Physics, 2008, 129, 054901.	1.2	29
51	Time correlations and the second entropy. Journal of Chemical Physics, 2007, 127, 044503.	1.2	2
52	Screening and strain in superionic conductors. Faraday Discussions, 2007, 134, 297-313.	1.6	2
53	Interpreting Size-Exclusion Data for Highly Branched Biopolymers by Reverse Monte Carlo Simulations. Biomacromolecules, 2007, 8, 455-463.	2.6	17
54	Toward a More General Solution to the Band-Broadening Problem in Size Separation of Polymers. Macromolecules, 2007, 40, 3477-3487.	2.2	33

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55	Nanoparticle Enhanced Conductivity in Organic Ionic Plastic Crystals:â€‰ Space Charge versus Strain Induced Defect Mechanism. Journal of Physical Chemistry C, 2007, 111, 11463-11468.	1.5	49
56	Theory of Multiple-Detection Size-Exclusion Chromatography of Complex Branched Polymers. Macromolecular Theory and Simulations, 2007, 16, 13-28.	0.6	93
57	Molecular weight distributions from size separation data for hyperbranched polymers. Journal of Polymer Science Part A, 2007, 45, 3112-3115.	2.5	24
58	Randomly Hyperbranched Polymers. Physical Review Letters, 2007, 98, 238301.	2.9	39
59	Role of Protein Flexibility in Ion Permeation: A Case Study in Gramicidin A. Biophysical Journal, 2006, 90, 2285-2296.	0.2	34
60	The Energy Landscape of a Fluorite-Structured Superionic Conductor. Journal of Physical Chemistry B, 2004, 108, 6634-6642.	1.2	16
61	Dynamical Arrest in Superionic Crystals and Supercooled Liquids. Journal of Physical Chemistry B, 2004, 108, 6624-6633.	1.2	22
62	Theoretical calculation of the structure of a polarizable-ionic fluid. Molecular Physics, 2003, 101, 1761-1779.	0.8	14
63	Induced-dipole contributions to the conductivity and dielectric response of molten ZnCl2. Journal of Chemical Physics, 2000, 113, 6782-6787.	1.2	19
64	Transition-State Theory Model for the Diffusion Coefficients of Small Penetrants in Glassy Polymers. Macromolecules, 1997, 30, 7296-7306.	2.2	69