Stephen A Wells

List of Publications by Year
in descending order

55 papers	1,725 citations	304368 22 h-index	288905 40 g-index
57 all docs	57 docs citations	57 times ranked	2044 citing authors

#	Article	IF	Citations
1	Stereoselective metabolism of chloramphenicol by bacteria isolated from wastewater, and the importance of stereochemistry in environmental risk assessments for antibiotics. Water Research, 2022, 217, 118415.	5.3	3
2	Determining the structure of zeolite frameworks at high pressures. CrystEngComm, 2021, 23, 5615-5623.	1.3	6
3	Using geometric simulation software â€˜GASPâ€™ to model conformational flexibility in a family of zinc metalâ€“organic frameworks. New Journal of Chemistry, 2021, 45, 8728-8737.	1.4	2
4	Cisplatin uptake and release in pH sensitive zeolitic imidazole frameworks. Journal of Chemical Physics, 2021, 154, 244703.	1.2	7
5	Structure and in silico simulations of a cold-active esterase reveals its prime cold-adaptation mechanism. Open Biology, 2021, 11, 210182.	1.5	10
6	Salt bridge impact on global rigidity and thermostability in thermophilic citrate synthase. Physical Biology, 2020, 17, 016002.	0.8	11
7	Monoclonal antibody stability can be usefully monitored using the excitation-energy-dependent fluorescence edge-shift. Biochemical Journal, 2020, 477, 3599-3612.	1.7	13
8	The steric influence of extra-framework cations on framework flexibility: an LTA case study. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 461-468.	0.4	9
9	Early stages of phase selection in MOF formation observed in molecular Monte Carlo simulations. RSC Advances, 2019, 9, 14382-14390.	1.7	8
10	TCRâ€induced alteration of primary MHC peptide anchor residue. European Journal of Immunology, 2019, 49, 1052-1066.	1.6	23
11	Intrinsic Flexibility of the EMT Zeolite Framework under Pressure. Molecules, 2019, 24, 641.	1.7	8
12	Exposing the Interplay Between Enzyme Turnover, Protein Dynamics, and the Membrane Environment in Monoamine Oxidase B. Biochemistry, 2019, 58, 2362-2372.	1.2	12
13	Pressure-induced symmetry changes in body-centred cubic zeolites. Royal Society Open Science, 2019, 6, 182158.	1.1	13
14	Structure and function of<scp>L</scp>-threonine-3-dehydrogenase from the parasitic protozoanTrypanosoma bruceirevealed by X-ray crystallography and geometric simulations. Acta Crystallographica Section D: Structural Biology, 2018, 74, 861-876.	1.1	8
15	In Silico and Structural Analyses Demonstrate That Intrinsic Protein Motions Guide T Cell Receptor Complementarity Determining Region Loop Flexibility. Frontiers in Immunology, 2018, 9, 674.	2.2	26
16	Mechanism of CO2 capture in nanostructured sodium amide encapsulated in porous silica. Surface and Coatings Technology, 2018, 350, 227-233.	2.2	7
17	Thermal stability, storage and release of proteins with tailored fit in silica. Scientific Reports, 2017, 7, 46568.	1.6	36
18	Evidence of Correlated Static Disorder in the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2017, 8, 2350-2356.	2.1	9

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19	Defining the flexibility window in ordered aluminosilicate zeolites. Royal Society Open Science, 2017, 4, 170757.	1.1	9
20	â€˜Something in the way she movesâ€™: The functional significance of flexibility in the multiple roles of protein disulfide isomerase (PDI). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 1383-1394.	1.1	58
21	A complete thermodynamic analysis of enzyme turnover links the free energy landscape to enzyme catalysis. FEBS Journal, 2017, 284, 2829-2842.	2.2	39
22	The flexibility and dynamics of protein disulfide isomerase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1776-1785.	1.5	24
23	Intrinsic flexibility of porous materials; theory, modelling and the flexibility window of the EMT zeolite framework. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 641-647.	0.5	12
24	Structure and Function in Homodimeric Enzymes: Simulations of Cooperative and Independent Functional Motions. PLoS ONE, 2015, 10, e0133372.	1.1	24
25	Characterization of Folding Cores in the Cyclophilin A-Cyclosporin A Complex. Biophysical Journal, 2015, 108, 1739-1746.	0.2	4
26	Flexibility windows in faujasite with explicit water and methanol extra-framework content. Dalton Transactions, 2015, 44, 5978-5984.	1.6	13
27	GASP: software for geometric simulations of flexibility in polyhedral and molecular framework structures. Molecular Simulation, 2015, 41, 1409-1421.	0.9	27
28	Structures of mesophilic and extremophilic citrate synthases reveal rigidity and flexibility for function. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2657-2670.	1.5	28
29	Geometric Simulation of Flexible Motion in Proteins. Methods in Molecular Biology, 2014, 1084, 173-192.	0.4	5
30	High-resolution NMR studies of structure and dynamics of human ERp27 indicate extensive interdomain flexibility. Biochemical Journal, 2013, 450, 321-332.	1.7	14
31	Flexibility windows and compression of monoclinic and orthorhombic silicalites. Physical Review B, 2012, 85, .	1.1	28
32	Framework flexibility and rational design of new zeolites for catalysis. Applied Petrochemical Research, 2012, 2, 69-72.	1.3	8
33	Exploring the Energy Landscapes of Protein Folding Simulations with Bayesian Computation. Biophysical Journal, 2012, 102, 878-886.	0.2	51
34	Template-Based Geometric Simulation of Flexible Frameworks. Materials, 2012, 5, 415-431.	1.3	17
35	Protein flexibility is key to cisplatin crosslinking in calmodulin. Protein Science, 2012, 21, 1269-1279.	3.1	36
36	Charge transport in cancer-related genes and early carcinogenesis. Computer Physics Communications, 2011, 182, 36-38.	3.0	10

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37	The ALS Nutrition/NIPPV Study: Design, feasibility, and initial results. Amyotrophic Lateral Sclerosis and Other Motor Neuron Disorders, 2011, 12, 17-25.	2.3	19
38	Compression behaviour and flexibility window of the analcime-like feldspathoids: experimental and theoretical findings. European Journal of Mineralogy, 2009, 21, 571-580.	0.4	22
39	MODELLING CHARGE TRANSPORT IN DNA USING TRANSFER MATRICES WITH DIAGONAL TERMS. International Journal of Modern Physics B, 2009, 23, 4138-4149.	1.0	13
40	Fitting Low-Resolution Cryo-EM Maps of Proteins Using Constrained Geometric Simulations. Biophysical Journal, 2008, 94, 1613-1621.	0.2	70
41	The origin of the compressibility anomaly in amorphous silica: a molecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 275210.	0.7	22
42	Docking of Photosystem I Subunit C Using a Constrained Geometric Simulation. Journal of the American Chemical Society, 2006, 128, 8803-8812.	6.6	32
43	Cation substitution and strain screening in framework structures: The role of rigid unit modes. Chemical Geology, 2006, 225, 213-221.	1.4	10
44	The flexibility window in zeolites. Nature Materials, 2006, 5, 962-965.	13.3	177
45	Structural evolution of zeolite levyne under hydrostatic and non-hydrostatic pressure: geometric modelling. Physics and Chemistry of Minerals, 2006, 33, 243-255.	0.3	22
46	Total scattering and reverse Monte Carlo study of the 105 K displacive phase transition in strontium titanate. Journal of Physics Condensed Matter, 2005, 17, S111-S124.	0.7	38
47	Constrained geometric simulation of diffusive motion in proteins. Physical Biology, 2005, 2, S127-S136.	0.8	166
48	Negative Thermal Expansion inZrW2O8: Mechanisms, Rigid Unit Modes, and Neutron Total Scattering. Physical Review Letters, 2005, 95, 255501.	2.9	164
49	Ionic diffusion in quartz studied by transport measurements, SIMS and atomistic simulations. Journal of Physics Condensed Matter, 2005, 17, 1099-1112.	0.7	18
50	Tetrahedral Distortion and Energetic Packing Penalty in â€œZeoliteâ€•Frameworks:Â Linked Phenomena?. Journal of Physical Chemistry B, 2005, 109, 14783-14785.	1.2	26
51	Li+ion motion in quartz and Î²-eucryptite studied by dielectric spectroscopy and atomistic simulations. Journal of Physics Condensed Matter, 2004, 16, 8173-8189.	0.7	36
52	Reverse Monte Carlo with geometric analysis â€“ RMC+GA. Journal of Applied Crystallography, 2004, 37, 536-544.	1.9	40
53	Finding best-fit polyhedral rotations with geometric algebra. Journal of Physics Condensed Matter, 2002, 14, 4567-4584.	0.7	45
54	Real-space rigid-unit-mode analysis of dynamic disorder in quartz, cristobalite and amorphous silica. Journal of Physics Condensed Matter, 2002, 14, 4645-4657.	0.7	43

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55	Formation of a metallic glass by thermal decomposition of Fe(CO)5. Physical Review Letters, 1985, 55, 410-413.	2.9	139