Stephen A Wells

List of Publications by Year
in descending order

55 papers	1,725 citations	304743 22 h-index	289244 40 g-index
57 all docs	57 docs citations	57 times ranked	2044 citing authors

#	Article	IF	Citations
1	The flexibility window in zeolites. Nature Materials, 2006, 5, 962-965.	27.5	177
2	Constrained geometric simulation of diffusive motion in proteins. Physical Biology, 2005, 2, S127-S136.	1.8	166
3	Negative Thermal Expansion inZrW2O8: Mechanisms, Rigid Unit Modes, and Neutron Total Scattering. Physical Review Letters, 2005, 95, 255501.	7.8	164
4	Formation of a metallic glass by thermal decomposition of Fe(CO)5. Physical Review Letters, 1985, 55, 410-413.	7.8	139
5	Fitting Low-Resolution Cryo-EM Maps of Proteins Using Constrained Geometric Simulations. Biophysical Journal, 2008, 94, 1613-1621.	0.5	70
6	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.	2.3	58
7	Exploring the Energy Landscapes of Protein Folding Simulations with Bayesian Computation. Biophysical Journal, 2012, 102, 878-886.	0.5	51
8	Finding best-fit polyhedral rotations with geometric algebra. Journal of Physics Condensed Matter, 2002, 14, 4567-4584.	1.8	45
9	Real-space rigid-unit-mode analysis of dynamic disorder in quartz, cristobalite and amorphous silica. Journal of Physics Condensed Matter, 2002, 14, 4645-4657.	1.8	43
10	Reverse Monte Carlo with geometric analysis â€“ RMC+GA. Journal of Applied Crystallography, 2004, 37, 536-544.	4.5	40
11	A complete thermodynamic analysis of enzyme turnover links the free energy landscape to enzyme catalysis. FEBS Journal, 2017, 284, 2829-2842.	4.7	39
12	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.	1.8	38
13	Li+ion motion in quartz and Î²-eucryptite studied by dielectric spectroscopy and atomistic simulations. Journal of Physics Condensed Matter, 2004, 16, 8173-8189.	1.8	36
14	Protein flexibility is key to cisplatin crosslinking in calmodulin. Protein Science, 2012, 21, 1269-1279.	7.6	36
15	Thermal stability, storage and release of proteins with tailored fit in silica. Scientific Reports, 2017, 7, 46568.	3.3	36
16	Docking of Photosystem I Subunit C Using a Constrained Geometric Simulation. Journal of the American Chemical Society, 2006, 128, 8803-8812.	13.7	32
17	Flexibility windows and compression of monoclinic and orthorhombic silicalites. Physical Review B, 2012, 85, .	3.2	28
18	Structures of mesophilic and extremophilic citrate synthases reveal rigidity and flexibility for function. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2657-2670.	2.6	28

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19	GASP: software for geometric simulations of flexibility in polyhedral and molecular framework structures. Molecular Simulation, 2015, 41, 1409-1421.	2.0	27
20	Tetrahedral Distortion and Energetic Packing Penalty in â€œZeoliteâ€•Frameworks:Â Linked Phenomena?. Journal of Physical Chemistry B, 2005, 109, 14783-14785.	2.6	26
21	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.	4.8	26
22	Structure and Function in Homodimeric Enzymes: Simulations of Cooperative and Independent Functional Motions. PLoS ONE, 2015, 10, e0133372.	2.5	24
23	The flexibility and dynamics of protein disulfide isomerase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1776-1785.	2.6	24
24	TCRâ€induced alteration of primary MHC peptide anchor residue. European Journal of Immunology, 2019, 49, 1052-1066.	2.9	23
25	Structural evolution of zeolite levyne under hydrostatic and non-hydrostatic pressure: geometric modelling. Physics and Chemistry of Minerals, 2006, 33, 243-255.	0.8	22
26	The origin of the compressibility anomaly in amorphous silica: a molecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 275210.	1.8	22
27	Compression behaviour and flexibility window of the analcime-like feldspathoids: experimental and theoretical findings. European Journal of Mineralogy, 2009, 21, 571-580.	1.3	22
28	The ALS Nutrition/NIPPV Study: Design, feasibility, and initial results. Amyotrophic Lateral Sclerosis and Other Motor Neuron Disorders, 2011, 12, 17-25.	2.1	19
29	Ionic diffusion in quartz studied by transport measurements, SIMS and atomistic simulations. Journal of Physics Condensed Matter, 2005, 17, 1099-1112.	1.8	18
30	Template-Based Geometric Simulation of Flexible Frameworks. Materials, 2012, 5, 415-431.	2.9	17
31	High-resolution NMR studies of structure and dynamics of human ERp27 indicate extensive interdomain flexibility. Biochemical Journal, 2013, 450, 321-332.	3.7	14
32	MODELLING CHARGE TRANSPORT IN DNA USING TRANSFER MATRICES WITH DIAGONAL TERMS. International Journal of Modern Physics B, 2009, 23, 4138-4149.	2.0	13
33	Flexibility windows in faujasite with explicit water and methanol extra-framework content. Dalton Transactions, 2015, 44, 5978-5984.	3.3	13
34	Pressure-induced symmetry changes in body-centred cubic zeolites. Royal Society Open Science, 2019, 6, 182158.	2.4	13
35	Monoclonal antibody stability can be usefully monitored using the excitation-energy-dependent fluorescence edge-shift. Biochemical Journal, 2020, 477, 3599-3612.	3.7	13
36	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.	1.1	12

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37	Exposing the Interplay Between Enzyme Turnover, Protein Dynamics, and the Membrane Environment in Monoamine Oxidase B. Biochemistry, 2019, 58, 2362-2372.	2.5	12
38	Salt bridge impact on global rigidity and thermostability in thermophilic citrate synthase. Physical Biology, 2020, 17, 016002.	1.8	11
39	Cation substitution and strain screening in framework structures: The role of rigid unit modes. Chemical Geology, 2006, 225, 213-221.	3.3	10
40	Charge transport in cancer-related genes and early carcinogenesis. Computer Physics Communications, 2011, 182, 36-38.	7.5	10
41	Structure and in silico simulations of a cold-active esterase reveals its prime cold-adaptation mechanism. Open Biology, 2021, 11, 210182.	3.6	10
42	Evidence of Correlated Static Disorder in the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2017, 8, 2350-2356.	4.6	9
43	Defining the flexibility window in ordered aluminosilicate zeolites. Royal Society Open Science, 2017, 4, 170757.	2.4	9
44	The steric influence of extra-framework cations on framework flexibility: an LTA case study. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 461-468.	0.8	9
45	Framework flexibility and rational design of new zeolites for catalysis. Applied Petrochemical Research, 2012, 2, 69-72.	1.3	8
46	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.	2.3	8
47	Early stages of phase selection in MOF formation observed in molecular Monte Carlo simulations. RSC Advances, 2019, 9, 14382-14390.	3.6	8
48	Intrinsic Flexibility of the EMT Zeolite Framework under Pressure. Molecules, 2019, 24, 641.	3.8	8
49	Mechanism of CO2 capture in nanostructured sodium amide encapsulated in porous silica. Surface and Coatings Technology, 2018, 350, 227-233.	4.8	7
50	Cisplatin uptake and release in pH sensitive zeolitic imidazole frameworks. Journal of Chemical Physics, 2021, 154, 244703.	3.0	7
51	Determining the structure of zeolite frameworks at high pressures. CrystEngComm, 2021, 23, 5615-5623.	2.6	6
52	Geometric Simulation of Flexible Motion in Proteins. Methods in Molecular Biology, 2014, 1084, 173-192.	0.9	5
53	Characterization of Folding Cores in the Cyclophilin A-Cyclosporin A Complex. Biophysical Journal, 2015, 108, 1739-1746.	0.5	4
54	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.	11.3	3

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55	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.	2.8	2