Jamshed Anwar

List of Publications by Year in descending order

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71 papers	4,028 citations	126708 33 h-index	118652 62 g-index
76 all docs	76 docs citations	76 times ranked	5131 citing authors

#	Article	IF	Citations
1	Modulating the Structure and Properties of Cell Membranes:â€‰ The Molecular Mechanism of Action of Dimethyl Sulfoxide. Journal of Physical Chemistry B, 2007, 111, 10453-10460.	1.2	354
2	Molecular Basis for Dimethylsulfoxide (DMSO) Action on Lipid Membranes. Journal of the American Chemical Society, 2006, 128, 13982-13983.	6.6	346
3	Structure of ice crystallized from supercooled water. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 1041-1045.	3.3	274
4	Uncovering Molecular Processes in Crystal Nucleation and Growth by Using Molecular Simulation. Angewandte Chemie - International Edition, 2011, 50, 1996-2013.	7.2	220
5	The Human Skin Barrier Is Organized as Stacked Bilayers of Fully Extended Ceramides with Cholesterol Molecules Associated with the Ceramide Sphingoid Moiety. Journal of Investigative Dermatology, 2012, 132, 2215-2225.	0.3	194
6	Defect-Mediated Trafficking across Cell Membranes: Insights from in Silico Modeling. Chemical Reviews, 2010, 110, 6077-6103.	23.0	171
7	The Permeability Enhancing Mechanism of DMSO in Ceramide Bilayers Simulated by Molecular Dynamics. Biophysical Journal, 2007, 93, 2056-2068.	0.2	152
8	Interaction of Ethanol with Biological Membranes: The Formation of Non-bilayer Structures within the Membrane Interior and their Significance. Journal of Physical Chemistry B, 2009, 113, 1983-1992.	1.2	144
9	Computer Simulation of Crystallization from Solution. Journal of the American Chemical Society, 1998, 120, 9600-9604.	6.6	125
10	Calculation of the melting point of NaCl by molecular simulation. Journal of Chemical Physics, 2003, 118, 728-735.	1.2	119
11	Crystallization of polymorphs: the effect of solvent. Journal Physics D: Applied Physics, 1993, 26, B90-B93.	1.3	108
12	Breaching the skin barrier â€" Insights from molecular simulation of model membranes. Advanced Drug Delivery Reviews, 2013, 65, 237-250.	6.6	96
13	Secondary Crystal Nucleation: Nuclei Breeding Factory Uncovered. Angewandte Chemie - International Edition, 2015, 54, 14681-14684.	7.2	92
14	Polymorphism of Sulfathiazole. Journal of Pharmaceutical Sciences, 1989, 78, 337-342.	1.6	86
15	Molecular dynamics simulation of a polysorbate 80 micelle in water. Soft Matter, 2011, 7, 2900.	1.2	79
16	Nanofiber-Based Delivery of Therapeutic Peptides to the Brain. ACS Nano, 2013, 7, 1016-1026.	7.3	77
17	Direct Calculation of Solid-Liquid Interfacial Free Energy for Molecular Systems: TIP4P Ice-Water Interface. Physical Review Letters, 2008, 100, 036104.	2.9	73
18	Nanocrystal Preparation: Low-Energy Precipitation Method Revisited. Crystal Growth and Design, 2013, 13, 2766-2777.	1.4	70

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19	Mode of Action and Design Rules for Additives That Modulate Crystal Nucleation. Angewandte Chemie - International Edition, 2009, 48, 1596-1600.	7.2	68
20	An Approach to Developing a Force Field for Molecular Simulation of Martensitic Phase Transitions between Phases with Subtle Differences in Energy and Structure. Journal of the American Chemical Society, 2004, 126, 396-405.	6.6	66
21	Challenges in molecular simulation of homogeneous ice nucleation. Journal of Physics Condensed Matter, 2008, 20, 494243.	0.7	59
22	The Riddle of Resorcinol Crystal Growth Revisited:Â Molecular Dynamics Simulations of Î±-Resorcinol Crystalâ^'Water Interface. Journal of the American Chemical Society, 1999, 121, 8583-8591.	6.6	53
23	Concerted Molecular Displacements in a Thermally-Induced Solid-State Transformation in Crystals of DL-Norleucine. Journal of the American Chemical Society, 2007, 129, 2542-2547.	6.6	51
24	Polymorphic phase transitions: Macroscopic theory and molecular simulation. Advanced Drug Delivery Reviews, 2017, 117, 47-70.	6.6	49
25	Synthesis and Characterization of Biodegradable Hydrogels for Oral Delivery of 5â€Fluorouracil Targeted to Colon: Screening with Preliminary In Vivo Studies. Advances in Polymer Technology, 2018, 37, 221-229.	0.8	49
26	Ab initiostructure determination of sulfathiazole polymorph V from synchrotron X-ray powder diffraction data. Journal of Applied Crystallography, 1999, 32, 436-441.	1.9	47
27	Why Do Some Molecules Form Hydrates or Solvates?. Crystal Growth and Design, 2018, 18, 1903-1908.	1.4	47
28	Ice I_hâ€“Water Interfacial Free Energy of Simple Water Models with Full Electrostatic Interactions. Journal of Chemical Theory and Computation, 2012, 8, 2383-2390.	2.3	45
29	Simulations of Skin Barrier Function: Free Energies of Hydrophobic and Hydrophilic Transmembrane Pores in Ceramide Bilayers. Biophysical Journal, 2008, 95, 4763-4771.	0.2	42
30	Kinetics of the Solid-State Phase Transformation of Form Î² to Î³ of Sulfanilamide Using Time-Resolved Energy-Dispersive X-ray Diffraction. Chemistry of Materials, 1996, 8, 1042-1051.	3.2	38
31	Interaction of Oleic Acid with Dipalmitoylphosphatidylcholine (DPPC) Bilayers Simulated by Molecular Dynamics. Journal of Physical Chemistry B, 2007, 111, 12748-12755.	1.2	37
32	Chemically Induced Phospholipid Translocation Across Biological Membranes. Langmuir, 2008, 24, 9656-9660.	1.6	36
33	Prediction of the Mechanical Behaviour of Crystalline Solids. Pharmaceutical Research, 2012, 29, 319-331.	1.7	36
34	Study of the effect of solvent on the morphology of crystals using molecular simulation: application to Î±-resorcinol and N-n-octyl-D-gluconamide. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 1023-1025.	1.7	33
35	Ion Transport through Chemically Induced Pores in Protein-Free Phospholipid Membranes. Journal of Physical Chemistry B, 2007, 111, 13379-13382.	1.2	33
36	Dielectric analysis of phosphorylcholine head group mobility in egg lecithin liposomes. Pharmaceutical Research, 1996, 13, 1181-1185.	1.7	29

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37	Robust and accurate method for free-energy calculation of charged molecular systems. Journal of Chemical Physics, 2005, 122, 224117.	1.2	29
38	Solubility prediction from first principles: a density of states approach. Physical Chemistry Chemical Physics, 2018, 20, 20981-20987.	1.3	26
39	CD-MOFs Crystal Transformation from Dense to Highly Porous Form for Efficient Drug Loading. Crystal Growth and Design, 2019, 19, 3888-3894.	1.4	24
40	DL-Norleucine: redetermination of structure and observations with synchrotron radiation Laue diffraction on heating towards transformation. Acta Crystallographica Section B: Structural Science, 1995, 51, 1059-1062.	1.8	21
41	Collective displacements in a molecular crystal polymorphic transformation. RSC Advances, 2013, 3, 12810.	1.7	19
42	Partitioning into Colloidal Structures of Fasted State Intestinal Fluid Studied by Molecular Dynamics Simulations. Langmuir, 2016, 32, 12732-12740.	1.6	19
43	Asymmetric Crystal Growth of Î±-Resorcinol from the Vapor Phase: Surface Reconstruction and Conformational Change Are the Culprits. Angewandte Chemie - International Edition, 2007, 46, 5537-5540.	7.2	18
44	The Molecular Mechanism of Î±-Resorcinolâ€™s Asymmetric Crystal Growth from the Melt. Crystal Growth and Design, 2015, 15, 4026-4031.	1.4	18
45	Solvent and additive interactions as determinants in the nucleation pathway: general discussion. Faraday Discussions, 2015, 179, 383-420.	1.6	18
46	The use of fast powder diffraction methods to study transformations. Journal of Materials Science Letters, 1990, 9, 436-439.	0.5	16
47	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE‹scp›ngine‹/scp›): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	1.2	15
48	Sizeâ€Đependent Phase Stability of a Molecular Nanocrystal: a Proxy for Investigating the Early Stages of Crystallization. Chemistry - A European Journal, 2011, 17, 11186-11192.	1.7	14
49	Investigations on Anticancer Potentials by DNA Binding and Cytotoxicity Studies for Newly Synthesized and Characterized Imidazolidine and Thiazolidine-Based Isatin Derivatives. Molecules, 2022, 27, 354.	1.7	14
50	Molecular dynamics simulations of granular compaction: The single granule case. Journal of Chemical Physics, 2003, 118, 4636-4648.	1.2	13
51	A molecular dynamics simulation study of the effects of defects on the transformation pressure of polymorphic phase transformations. Journal of Chemical Physics, 1996, 105, 3215-3218.	1.2	12
52	Two-Step Nucleation Rather than Self-Poisoning: An Unexpected Mechanism of Asymmetrical Molecular Crystal Growth. Crystal Growth and Design, 2015, 15, 5118-5123.	1.4	12
53	Nanocrystal Recovery by Use of Carrier Particles. Crystal Growth and Design, 2014, 14, 1003-1009.	1.4	11
54	Secondary Crystal Nucleation: Nuclei Breeding Factory Uncovered. Angewandte Chemie, 2015, 127, 14894-14897.	1.6	11

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55	Molecular self-assembly and clustering in nucleation processes: general discussion. Faraday Discussions, 2015, 179, 155-197.	1.6	10
56	Molecular Dynamics Simulations of Granular Compaction. Chemistry of Materials, 2003, 15, 3417-3430.	3.2	9
57	Evaluation and Optimization of a Force Field for Crystalline Forms of Mannitol and Sorbitol. Journal of Physical Chemistry B, 2010, 114, 429-436.	1.2	9
58	Free energies of crystals computed using Einstein crystal with fixed center of mass and differing spring constants. Journal of Chemical Physics, 2021, 154, 164509.	1.2	9
59	Kinetics of phase transformations in crystals of drug compounds using time-resolved powder x-ray diffraction. Phase Transitions, 1992, 39, 3-11.	0.6	7
60	Solubility prediction for a soluble organic molecule via chemical potentials from density of states. Journal of Chemical Physics, 2019, 151, 184113.	1.2	7
61	Heparin-Assisted Amyloidogenesis Uncovered through Molecular Dynamics Simulations. ACS Omega, 2022, 7, 15132-15144.	1.6	7
62	Analysis of time-resolved powder diffraction data using a pattern-decomposition method with restraints. Journal of Applied Crystallography, 1993, 26, 413-421.	1.9	5
63	Investigating effect of mutation on structure and function of G6PD enzyme: a comparative molecular dynamics simulation study. PeerJ, 2022, 10, e12984.	0.9	4
64	An optimized force field for crystalline phases of resorcinol. CrystEngComm, 2008, , .	1.3	3
65	Conceptual, self-assembling graphene nanocontainers. Nanoscale, 2015, 7, 12104-12108.	2.8	3
66	Toward the Noninvasive Diagnosis of Alzheimerâ€™s Disease: Molecular Basis for the Specificity of Curcumin for Fibrillar Amyloid-Î². ACS Omega, 2022, 7, 22032-22038.	1.6	3
67	Towards crystal engineering: Probing crystallization processes by computer simulation. Journal of Pharmacy and Pharmacology, 2011, 50, 51-51.	1.2	2
68	Solidâ€“solid phase equilibria in the NaClâ€“KCl system. Journal of Chemical Physics, 2020, 152, 144109.	1.2	2
69	Computer simulation of crystal-liquid interface: application to wettability of solids. Pharmaceutical Research, 1996, 13, 1003-1007.	1.7	1
70	Towards crystal engineering: probing crystallization processes by computer simulation. Journal of Pharmacy and Pharmacology, 2011, 50, ii-ii.	1.2	0
71	Directing self-assembly to grow adaptive physical structures. International Journal of Rapid Manufacturing, 2017, 6, 114.	0.5	0