## Feng Ding

## List of Publications by Year in descending order

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28190 43802 9,858 168 55 91 citations h-index g-index papers 178 178 178 9801 docs citations times ranked citing authors all docs

| #  | Article                                                                                                                                                             | IF   | CITATIONS |
|----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----------|
| 1  | Automated minimization of steric clashes in protein structures. Proteins: Structure, Function and Bioinformatics, 2011, 79, 261-270.                                | 1.5  | 372       |
| 2  | Eris: an automated estimator of protein stability. Nature Methods, 2007, 4, 466-467.                                                                                | 9.0  | 355       |
| 3  | Ab Initio Folding of Proteins with All-Atom Discrete Molecular Dynamics. Structure, 2008, 16, 1010-1018.                                                            | 1.6  | 287       |
| 4  | Topological determinants of protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 8637-8641.                  | 3.3  | 278       |
| 5  | Implications of peptide assemblies in amyloid diseases. Chemical Society Reviews, 2017, 46, 6492-6531.                                                              | 18.7 | 262       |
| 6  | Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. Nature Reviews Drug Discovery, 2009, 8, 455-463.                          | 21.5 | 260       |
| 7  | Ab initio RNA folding by discrete molecular dynamics: From structure prediction to folding mechanisms. Rna, 2008, 14, 1164-1173.                                    | 1.6  | 258       |
| 8  | Mechanism for the ?-helix to ?-hairpin transition. Proteins: Structure, Function and Bioinformatics, 2003, 53, 220-228.                                             | 1.5  | 252       |
| 9  | <i>RNA-Puzzles</i> : A CASP-like evaluation of RNA three-dimensional structure prediction. Rna, 2012, 18, 610-625.                                                  | 1.6  | 241       |
| 10 | iFoldRNA: three-dimensional RNA structure prediction and folding. Bioinformatics, 2008, 24, 1951-1952.                                                              | 1.8  | 200       |
| 11 | Molecular Dynamics Simulation of Amyloid $\hat{l}^2$ Dimer Formation. Biophysical Journal, 2004, 87, 2310-2321.                                                     | 0.2  | 194       |
| 12 | Discrete Molecular Dynamics: An Efficient And Versatile Simulation Method For Fine Protein Characterization. Journal of Physical Chemistry B, 2012, 116, 8375-8382. | 1.2  | 179       |
| 13 | Emergence of Protein Fold Families through Rational Design. PLoS Computational Biology, 2006, 2, e85.                                                               | 1.5  | 177       |
| 14 | Engineered allosteric activation of kinases in living cells. Nature Biotechnology, 2010, 28, 743-747.                                                               | 9.4  | 177       |
| 15 | <i>RNA-Puzzles</i> Round II: assessment of RNA structure prediction programs applied to three large RNA structures. Rna, 2015, 21, 1066-1084.                       | 1.6  | 161       |
| 16 | RNA-Puzzles Round III: 3D RNA structure prediction of five riboswitches and one ribozyme. Rna, 2017, 23, 655-672.                                                   | 1.6  | 158       |
| 17 | Molecular Dynamics Simulation of the SH3 Domain Aggregation Suggests a Generic Amyloidogenesis Mechanism. Journal of Molecular Biology, 2002, 324, 851-857.         | 2.0  | 157       |
| 18 | Modeling Backbone Flexibility Improves Protein Stability Estimation. Structure, 2007, 15, 1567-1576.                                                                | 1.6  | 147       |

| #  | Article                                                                                                                                                                                                               | IF   | Citations |
|----|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----------|
| 19 | Direct Molecular Dynamics Observation of Protein Folding Transition State Ensemble. Biophysical Journal, 2002, 83, 3525-3532.                                                                                         | 0.2  | 133       |
| 20 | Inhibition of amyloid beta toxicity in zebrafish with a chaperone-gold nanoparticle dual strategy. Nature Communications, 2019, 10, 3780.                                                                             | 5.8  | 132       |
| 21 | Dynamical roles of metal ions and the disulfide bond in Cu, Zn superoxide dismutase folding and aggregation. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 19696-19701. | 3.3  | 131       |
| 22 | Folding Trp-Cage to NMR Resolution Native Structure Using a Coarse-Grained Protein Model.<br>Biophysical Journal, 2005, 88, 147-155.                                                                                  | 0.2  | 130       |
| 23 | Direct observation of a single nanoparticle–ubiquitin corona formation. Nanoscale, 2013, 5, 9162.                                                                                                                     | 2.8  | 116       |
| 24 | Rational design of a ligand-controlled protein conformational switch. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6800-6804.                                          | 3.3  | 111       |
| 25 | Multiscale Modeling of Nucleosome Dynamics. Biophysical Journal, 2007, 92, 1457-1470.                                                                                                                                 | 0.2  | 104       |
| 26 | Stabilizing Off-pathway Oligomers by Polyphenol Nanoassemblies for IAPP Aggregation Inhibition. Scientific Reports, 2016, 6, 19463.                                                                                   | 1.6  | 104       |
| 27 | On the significance of an RNA tertiary structure prediction. Rna, 2010, 16, 1340-1349.                                                                                                                                | 1.6  | 103       |
| 28 | Graphene quantum dots against human IAPP aggregation and toxicity <i>in vivo</i> . Nanoscale, 2018, 10, 19995-20006.                                                                                                  | 2.8  | 100       |
| 29 | RNA-Puzzles Round IV: 3D structure predictions of four ribozymes and two aptamers. Rna, 2020, 26, 982-995.                                                                                                            | 1.6  | 100       |
| 30 | Inhibition of hIAPP Amyloid Aggregation and Pancreatic $\hat{l}^2$ -Cell Toxicity by OH-Terminated PAMAM Dendrimer. Small, 2016, 12, 1615-1626.                                                                       | 5.2  | 99        |
| 31 | Chemical and Biophysical Signatures of the Protein Corona in Nanomedicine. Journal of the American Chemical Society, 2022, 144, 9184-9205.                                                                            | 6.6  | 98        |
| 32 | Molecular Origin of Polyglutamine Aggregation in Neurodegenerative Diseases. PLoS Computational Biology, 2005, 1, e30.                                                                                                | 1.5  | 92        |
| 33 | Discrete molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 80-92.                                                                                                        | 6.2  | 91        |
| 34 | Protein folding: Then and now. Archives of Biochemistry and Biophysics, 2008, 469, 4-19.                                                                                                                              | 1.4  | 88        |
| 35 | Mitigation of Amyloidosis with Nanomaterials. Advanced Materials, 2020, 32, e1901690.                                                                                                                                 | 11.1 | 87        |
| 36 | Polyglutamine Induced Misfolding of Huntingtin Exon1 is Modulated by the Flanking Sequences. PLoS Computational Biology, 2010, 6, e1000772.                                                                           | 1.5  | 86        |

| #  | Article                                                                                                                                                                                    | IF  | CITATIONS |
|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------|
| 37 | Rapid Flexible Docking Using a Stochastic Rotamer Library of Ligands. Journal of Chemical Information and Modeling, 2010, 50, 1623-1632.                                                   | 2.5 | 80        |
| 38 | Structural and Dynamic Determinants of Protein-Peptide Recognition. Structure, 2011, 19, 1837-1845.                                                                                        | 1.6 | 79        |
| 39 | Direct Observation of Protein Folding, Aggregation, and a Prion-like Conformational Conversion.<br>Journal of Biological Chemistry, 2005, 280, 40235-40240.                                | 1.6 | 77        |
| 40 | Three-dimensional RNA structure refinement by hydroxyl radical probing. Nature Methods, 2012, 9, 603-608.                                                                                  | 9.0 | 77        |
| 41 | Discrete molecular dynamics simulations of peptide aggregation. Physical Review E, 2004, 69, 041908.                                                                                       | 0.8 | 74        |
| 42 | Local Unfolding of Cu, Zn Superoxide Dismutase Monomer Determines the Morphology of Fibrillar Aggregates. Journal of Molecular Biology, 2012, 421, 548-560.                                | 2.0 | 74        |
| 43 | Simple but predictive protein models. Trends in Biotechnology, 2005, 23, 450-455.                                                                                                          | 4.9 | 73        |
| 44 | Topological Determinants of Protein Domain Swapping. Structure, 2006, 14, 5-14.                                                                                                            | 1.6 | 73        |
| 45 | Fast complementation of split fluorescent protein triggered by DNA hybridization. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 2052-2056.   | 3.3 | 73        |
| 46 | Reconstruction of the src-SH3 Protein Domain Transition State Ensemble using Multiscale Molecular Dynamics Simulations. Journal of Molecular Biology, 2005, 350, 1035-1050.                | 2.0 | 72        |
| 47 | Graphene oxide inhibits hIAPP amyloid fibrillation and toxicity in insulin-producing NIT-1 cells. Physical Chemistry Chemical Physics, 2016, 18, 94-100.                                   | 1.3 | 70        |
| 48 | Native-like RNA Tertiary Structures Using a Sequence-Encoded Cleavage Agent and Refinement by Discrete Molecular Dynamics. Journal of the American Chemical Society, 2009, 131, 2541-2546. | 6.6 | 65        |
| 49 | Harnessing a Physiologic Mechanism for siRNA Delivery With Mimetic Lipoprotein Particles. Molecular<br>Therapy, 2012, 20, 1582-1589.                                                       | 3.7 | 65        |
| 50 | Star Polymers Reduce Islet Amyloid Polypeptide Toxicity via Accelerated Amyloid Aggregation. Biomacromolecules, 2017, 18, 4249-4260.                                                       | 2.6 | 65        |
| 51 | New Insights into FAK Signaling and Localization Based on Detection of a FAT Domain Folding Intermediate. Structure, 2004, 12, 2161-2171.                                                  | 1.6 | 62        |
| 52 | î²-barrel Oligomers as Common Intermediates of Peptides Self-Assembling into Cross-β Aggregates.<br>Scientific Reports, 2018, 8, 10353.                                                    | 1.6 | 62        |
| 53 | Competitive Binding of Natural Amphiphiles with Graphene Derivatives. Scientific Reports, 2013, 3, 2273.                                                                                   | 1.6 | 61        |
| 54 | Folding of Cu, Zn Superoxide Dismutase and Familial Amyotrophic Lateral Sclerosis. Journal of Molecular Biology, 2003, 334, 515-525.                                                       | 2.0 | 59        |

| #  | Article                                                                                                                                                                                                          | IF  | Citations |
|----|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------|
| 55 | Scaling Behavior and Structure of Denatured Proteins. Structure, 2005, 13, 1047-1054.                                                                                                                            | 1.6 | 58        |
| 56 | Mitigating Human IAPP Amyloidogenesis In Vivo with Chiral Silica Nanoribbons. Small, 2018, 14, e1802825.                                                                                                         | 5.2 | 57        |
| 57 | Contrasting effects of nanoparticle–protein attraction on amyloid aggregation. RSC Advances, 2015, 5, 105489-105498.                                                                                             | 1.7 | 56        |
| 58 | Inhibition of IAPP aggregation by insulin depends on the insulin oligomeric state regulated by zinc ion concentration. Scientific Reports, 2015, 5, 8240.                                                        | 1.6 | 50        |
| 59 | Cofibrillization of Pathogenic and Functional Amyloid Proteins with Gold Nanoparticles against Amyloidogenesis. Biomacromolecules, 2017, 18, 4316-4322.                                                          | 2.6 | 50        |
| 60 | Amyloid Selfâ€Assembly of hIAPP8â€20 via the Accumulation of Helical Oligomers, αâ€Helix to βâ€Sheet Transition, and Formation of βâ€Barrel Intermediates. Small, 2019, 15, e1805166.                            | 5.2 | 49        |
| 61 | Interaction of firefly luciferase and silver nanoparticles and its impact on enzyme activity.<br>Nanotechnology, 2013, 24, 345101.                                                                               | 1.3 | 47        |
| 62 | Amphiphilic surface chemistry of fullerenols is necessary for inhibiting the amyloid aggregation of alpha-synuclein NACore. Nanoscale, 2019, 11, 11933-11945.                                                    | 2.8 | 47        |
| 63 | Accelerated Amyloid Beta Pathogenesis by Bacterial Amyloid FapC. Advanced Science, 2020, 7, 2001299.                                                                                                             | 5.6 | 47        |
| 64 | Novel application of a perturbed photonic crystal: High-quality filter. Applied Physics Letters, 1997, 71, 2889-2891.                                                                                            | 1.5 | 46        |
| 65 | Gaia: automated quality assessment of protein structure models. Bioinformatics, 2011, 27, 2209-2215.                                                                                                             | 1.8 | 44        |
| 66 | Nucleation of $\hat{l}^2$ -rich oligomers and $\hat{l}^2$ -barrels in the early aggregation of human islet amyloid polypeptide. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2019, 1865, 434-444. | 1.8 | 44        |
| 67 | Spontaneous formation of β-sheet nano-barrels during the early aggregation of Alzheimer's amyloid beta. Nano Today, 2021, 38, 101125.                                                                            | 6.2 | 44        |
| 68 | Structural and Thermodynamic Effects of Post-translational Modifications in Mutant and Wild Type Cu, Zn Superoxide Dismutase. Journal of Molecular Biology, 2011, 408, 555-567.                                  | 2.0 | 43        |
| 69 | Computational approaches to understanding protein aggregation in neurodegeneration. Journal of Molecular Cell Biology, 2014, 6, 104-115.                                                                         | 1.5 | 43        |
| 70 | NanoEHS beyond toxicity – focusing on biocorona. Environmental Science: Nano, 2017, 4, 1433-1454.                                                                                                                | 2.2 | 43        |
| 71 | Distinct oligomerization and fibrillization dynamics of amyloid core sequences of amyloid-beta and islet amyloid polypeptide. Physical Chemistry Chemical Physics, 2017, 19, 28414-28423.                        | 1.3 | 43        |
| 72 | Active Nuclear Receptors Exhibit Highly Correlated AF-2 Domain Motions. PLoS Computational Biology, 2008, 4, e1000111.                                                                                           | 1.5 | 42        |

| #  | Article                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | IF           | Citations |
|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|-----------|
| 73 | Effect of fullerenol surface chemistry on nanoparticle binding-induced protein misfolding.<br>Nanoscale, 2014, 6, 8340-8349.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 2.8          | 41        |
| 74 | Identifying weak interdomain interactions that stabilize the supertertiary structure of the N-terminal tandem PDZ domains of PSD-95. Nature Communications, 2018, 9, 3724.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 5.8          | 41        |
| 75 | Understanding Effects of PAMAM Dendrimer Size and Surface Chemistry on Serum Protein Binding with Discrete Molecular Dynamics Simulations. ACS Sustainable Chemistry and Engineering, 2018, 6, 11704-11715.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 3.2          | 41        |
| 76 | The Length Dependence of the PolyQ-mediated Protein Aggregation. Journal of Biological Chemistry, 2007, 282, 25487-25492.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 1.6          | 40        |
| 77 | PAMAM Dendrimers and Graphene: Materials for Removing Aromatic Contaminants from Water. Environmental Science & Environmental | 4.6          | 40        |
| 78 | Islet Amyloid Polypeptide Promotes Amyloid-Beta Aggregation by Binding-Induced Helix-Unfolding of the Amyloidogenic Core. ACS Chemical Neuroscience, 2018, 9, 967-975.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 1.7          | 39        |
| 79 | Profiling the Serum Protein Corona of Fibrillar Human Islet Amyloid Polypeptide. ACS Nano, 2018, 12, 6066-6078.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 7.3          | 39        |
| 80 | Multiple Folding Pathways of the SH3 Domain. Biophysical Journal, 2004, 87, 521-533.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 0.2          | 38        |
| 81 | Modulating protein amyloid aggregation with nanomaterials. Environmental Science: Nano, 2017, 4, 1772-1783.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 2.2          | 38        |
| 82 | Incorporating Backbone Flexibility in MedusaDock Improves Ligand-Binding Pose Prediction in the CSAR2011 Docking Benchmark. Journal of Chemical Information and Modeling, 2013, 53, 1871-1879.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 2.5          | 37        |
| 83 | Binding of cytoskeletal proteins with silver nanoparticles. RSC Advances, 2013, 3, 22002.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 1.7          | 36        |
| 84 | Submillisecond Elastic Recoil Reveals Molecular Origins of Fibrin Fiber Mechanics. Biophysical Journal, 2013, 104, 2671-2680.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.2          | 35        |
| 85 | Nanoscale inhibition of polymorphic and ambidextrous IAPP amyloid aggregation with small molecules. Nano Research, 2018, 11, 3636-3647.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 5.8          | 35        |
| 86 | A structural model reveals energy transduction in dynein. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 18540-18545.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 3.3          | 34        |
| 87 | Effects of Protein Corona on IAPP Amyloid Aggregation, Fibril Remodelling, and Cytotoxicity. Scientific Reports, 2017, 7, 2455.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 1.6          | 34        |
| 88 | Graphene quantum dots rescue protein dysregulation of pancreatic $\hat{l}^2$ -cells exposed to human islet amyloid polypeptide. Nano Research, 2019, 12, 2827-2834.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 5 <b>.</b> 8 | 34        |
| 89 | Amyloid Aggregation under the Lens of Liquid–Liquid Phase Separation. Journal of Physical Chemistry<br>Letters, 2021, 12, 368-378.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 2.1          | 34        |
| 90 | Synthesis and in vitro properties of iron oxide nanoparticles grafted with brushed phosphorylcholine and polyethylene glycol. Polymer Chemistry, 2016, 7, 1931-1944.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 1.9          | 32        |

| #   | Article                                                                                                                                                                          | IF  | Citations |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------|
| 91  | Amyloidosis inhibition, a new frontier of the protein corona. Nano Today, 2020, 35, 100937.                                                                                      | 6.2 | 32        |
| 92  | Robust and Generic RNA Modeling Using Inferred Constraints: A Structure for the Hepatitis C Virus IRES Pseudoknot Domain. Biochemistry, 2010, 49, 4931-4933.                     | 1.2 | 31        |
| 93  | Structural Basis for μ-Opioid Receptor Binding and Activation. Structure, 2011, 19, 1683-1690.                                                                                   | 1.6 | 30        |
| 94  | Thermostability and reversibility of silver nanoparticle–protein binding. Physical Chemistry Chemical Physics, 2015, 17, 1728-1739.                                              | 1.3 | 30        |
| 95  | Parallel Folding Pathways in the SH3 Domain Protein. Journal of Molecular Biology, 2007, 373, 1348-1360.                                                                         | 2.0 | 29        |
| 96  | Nâ€ŧerminal strands of filamin Ig domains act as a conformational switch under biological forces. Proteins: Structure, Function and Bioinformatics, 2010, 78, 12-24.             | 1.5 | 29        |
| 97  | iFold: a platform for interactive folding simulations of proteins. Bioinformatics, 2006, 22, 2693-2694.                                                                          | 1.8 | 27        |
| 98  | Promotion or Inhibition of Islet Amyloid Polypeptide Aggregation by Zinc Coordination Depends on Its Relative Concentration. Biochemistry, 2015, 54, 7335-7344.                  | 1.2 | 27        |
| 99  | Structures and dynamics of $\hat{l}^2$ -barrel oligomer intermediates of amyloid-beta $16$ -22 aggregation. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1687-1697. | 1.4 | 27        |
| 100 | Single-Molecular Heteroamyloidosis of Human Islet Amyloid Polypeptide. Nano Letters, 2019, 19, 6535-6546.                                                                        | 4.5 | 27        |
| 101 | Hybrid Dynamics Simulation Engine for Metalloproteins. Biophysical Journal, 2012, 103, 767-776.                                                                                  | 0.2 | 26        |
| 102 | Nanosilver Mitigates Biofilm Formation via FapC Amyloidosis Inhibition. Small, 2020, 16, e1906674.                                                                               | 5.2 | 26        |
| 103 | G Protein Mono-ubiquitination by the Rsp5 Ubiquitin Ligase. Journal of Biological Chemistry, 2009, 284, 8940-8950.                                                               | 1.6 | 25        |
| 104 | Inhibition of Amyloid Aggregation and Toxicity with Janus Iron Oxide Nanoparticles. Chemistry of Materials, 2021, 33, 6484-6500.                                                 | 3.2 | 25        |
| 105 | Physical and toxicological profiles of human IAPP amyloids and plaques. Science Bulletin, 2019, 64, 26-35.                                                                       | 4.3 | 24        |
| 106 | Misfolding and Self-Assembly Dynamics of Microtubule-Binding Repeats of the Alzheimer-Related Protein Tau. Journal of Chemical Information and Modeling, 2021, 61, 2916-2925.    | 2.5 | 24        |
| 107 | Fidelity of the Protein Structure Reconstruction from Inter-Residue Proximity Constraints. Journal of Physical Chemistry B, 2007, 111, 7432-7438.                                | 1.2 | 23        |
| 108 | Elevated amyloidoses of human IAPP and amyloid beta by lipopolysaccharide and their mitigation by carbon quantum dots. Nanoscale, 2020, 12, 12317-12328.                         | 2.8 | 23        |

| #   | Article                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | IF  | CITATIONS |
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| 109 | Dynamic Protein Corona of Gold Nanoparticles with an Evolving Morphology. ACS Applied Materials & Lamp; Interfaces, 2021, 13, 58238-58251.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 4.0 | 23        |
| 110 | Mechanistic Insights from Discrete Molecular Dynamics Simulations of Pesticide–Nanoparticle Interactions. Environmental Science & Environmental Sci | 4.6 | 22        |
| 111 | Ultrasmall Molybdenum Disulfide Quantum Dots Cage Alzheimer's Amyloid Beta to Restore Membrane Fluidity. ACS Applied Materials & Interfaces, 2021, 13, 29936-29948.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | 4.0 | 22        |
| 112 | A Framework of Paracellular Transport via Nanoparticlesâ€Induced Endothelial Leakiness. Advanced Science, 2021, 8, e2102519.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 5.6 | 22        |
| 113 | Structure–Function Relationship of PAMAM Dendrimers as Robust Oil Dispersants. Environmental Science & Environmental Scienc | 4.6 | 21        |
| 114 | A Thermodynamics Model for the Emergence of a Stripeâ€like Binary SAM on a Nanoparticle Surface. Small, 2015, 11, 4894-4899.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 5.2 | 21        |
| 115 | Probing the modulated formation of gold nanoparticles–beta-lactoglobulin corona complexes and their applications. Nanoscale, 2017, 9, 17758-17769.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 2.8 | 21        |
| 116 | Zinc-coordination and C-peptide complexation: a potential mechanism for the endogenous inhibition of IAPP aggregation. Chemical Communications, 2017, 53, 9394-9397.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 2.2 | 21        |
| 117 | Probing protein aggregation using discrete molecular dynamics. Frontiers in Bioscience - Landmark, 2008, Volume, 4795.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 3.0 | 21        |
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