Irene Yarovsky

List of Publications by Year
in descending order

169 papers	5,765 citations	76031 42 h-index	116156 66 g-index
171 all docs	171 docs citations	171 times ranked	7965 citing authors

#	Article	IF	Citations
1	Modular assembly of superstructures from polyphenol-functionalized building blocks. Nature Nanotechnology, 2016, 11, 1105-1111.	15.6	337
2	Computer simulation of structure and properties of crosslinked polymers: application to epoxy resins. Polymer, 2002, 43, 963-969.	1.8	306
3	Density functional theory study of the relaxation and energy of iron surfaces. Surface Science, 2002, 513, 389-398.	0.8	154
4	Ordering Surfaces on the Nanoscale: Implications for Protein Adsorption. Journal of the American Chemical Society, 2011, 133, 1438-1450.	6.6	151
5	Density-functional theory studies of pyrite FeS2() and () surfaces. Surface Science, 2002, 513, 511-524.	0.8	144
6	Application of numerical basis sets to hydrogen bonded systems: A density functional theory study. Journal of Chemical Physics, 2005, 122, 144102.	1.2	122
7	Hybrid approach for generating realistic amorphous carbon structure using metropolis and reverse Monte Carlo. Molecular Simulation, 2002, 28, 927-938.	0.9	116
8	Nanomaterials in biological environment: a review of computer modelling studies. European Biophysics Journal, 2011, 40, 103-115.	1.2	108
9	ZnO Nanostructures for Gas Sensing: Interaction of NO₂, NO, O, and N with the ZnO(101Ì…0) Surface. Journal of Physical Chemistry C, 2010, 114, 10881-10893.	1.5	101
10	Surface enhanced Raman scattering artificial nose for high dimensionality fingerprinting. Nature Communications, 2020, 11, 207.	5.8	93
11	Influence of the Chain Length and Surface Density on the Conformation and Mobility of n-Alkyl Ligands Chemically Immobilized onto a Silica Surface. Analytical Chemistry, 1995, 67, 2145-2153.	3.2	87
12	Electric Field Effects on Insulin Chain-B Conformation. Journal of Physical Chemistry B, 2005, 109, 22641-22648.	1.2	87
13	Density-functional theory studies of pyrite FeS2 () and () surfaces. Surface Science, 2002, 520, 111-119.	0.8	82
14	Direct dry transfer of chemical vapor deposition graphene to polymeric substrates. Carbon, 2015, 83, 224-231.	5.4	82
15	Hydration Layer Structure of Biofouling-Resistant Nanoparticles. ACS Nano, 2018, 12, 11610-11624.	7.3	70
16	Adsorption of NO₂ on Oxygen Deficient ZnO(21Ì…1Ì…0) for Gas Sensing Applications: A DFT Study. Journal of Physical Chemistry C, 2010, 114, 16603-16610.	1.5	67
17	Effect of Frequency on Insulin Response to Electric Field Stress. Journal of Physical Chemistry B, 2007, 111, 5748-5756.	1.2	66
18	Performance of Numerical Basis Set DFT for Aluminum Clusters. Journal of Physical Chemistry A, 2008, 112, 9835-9844.	1.1	66

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19	Particle engineering enabled by polyphenol-mediated supramolecular networks. Nature Communications, 2020, 11, 4804.	5.8	65
20	First-principles studies of the structural and electronic properties of pyriteFeS2. Physical Review B, 2002, 65, .	1.1	64
21	First-principles study of metallic iron interfaces. Surface Science, 2002, 501, 261-269.	0.8	64
22	Cobalt Phosphate Nanostructures for Non-Enzymatic Glucose Sensing at Physiological pH. ACS Applied Materials & Interfaces, 2018, 10, 42786-42795.	4.0	64
23	Influence of Ionic Strength on the Deposition of Metalâ€“Phenolic Networks. Langmuir, 2017, 33, 10616-10622.	1.6	61
24	Dissociative Adsorption of Hydrogen Molecule on Aluminum Clusters: Effect of Charge and Doping. Journal of Physical Chemistry A, 2009, 113, 2565-2571.	1.1	59
25	Understanding and Designing the Goldâ€“Bio Interface: Insights from Simulations. Small, 2016, 12, 2395-2418.	5.2	58
26	Structural analysis of carbonaceous solids using an adapted reverse Monte Carlo algorithm. Carbon, 2003, 41, 2403-2411.	5.4	55
27	Microstructure of an industrial char by diffraction techniques and Reverse Monte Carlo modelling. Carbon, 2004, 42, 2457-2469.	5.4	55
28	Stereospecific Cyclic Poly(methyl methacrylate) and Its Topologyâ€Guided Hierarchically Controlled Supramolecular Assemblies. Angewandte Chemie - International Edition, 2014, 53, 459-464.	7.2	55
29	Protein flexibility: Multiple molecular dynamics simulations of insulin chain B. Biophysical Chemistry, 2006, 119, 146-157.	1.5	54
30	Surface Dynamics and Ligandâ€“Core Interactions of Quantum Sized Photoluminescent Gold Nanoclusters. Journal of the American Chemical Society, 2018, 140, 18217-18226.	6.6	54
31	DFT study of hydrogen adsorption on Al13clusters. Molecular Simulation, 2005, 31, 475-481.	0.9	53
32	Systematic Comparison of Empirical Forcefields for Molecular Dynamic Simulation of Insulin. Journal of Physical Chemistry B, 2008, 112, 11137-11146.	1.2	53
33	Molecular mapping of poly(methyl methacrylate) super-helix stereocomplexes. Chemical Science, 2015, 6, 1370-1378.	3.7	50
34	Investigation of Lignin-water interactions by molecular simulation. Molecular Simulation, 2002, 28, 981-991.	0.9	49
35	Adsorption of NO and NO2 on the ZnO() surface: A DFT study. Surface Science, 2009, 603, 3389-3399.	0.8	49
36	Dimensionality of Carbon Nanomaterials Determines the Binding and Dynamics of Amyloidogenic Peptides: Multiscale Theoretical Simulations. PLoS Computational Biology, 2013, 9, e1003360.	1.5	49

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37	Exploring the Folding Free Energy Landscape of Insulin Using Bias Exchange Metadynamics. Journal of Physical Chemistry B, 2009, 113, 3556-3564.	1.2	48
38	Amphiphilic amino acids: a key to adsorbing proteins to nanopatterned surfaces?. Chemical Science, 2013, 4, 928-937.	3.7	48
39	Electromagnetic-field effects on structure and dynamics of amyloidogenic peptides. Journal of Chemical Physics, 2016, 144, 085101.	1.2	46
40	Atomistic Simulation of Interfaces in Materials: Theory and Applications. Australian Journal of Physics, 1997, 50, 407.	0.6	45
41	A Structural Model for Apolipoprotein C-II Amyloid Fibrils: Experimental Characterization and Molecular Dynamics Simulations. Journal of Molecular Biology, 2011, 405, 1246-1266.	2.0	45
42	Density functional theory study of hydrogen adsorption onAl12cages. Physical Review B, 2007, 75, .	1.1	44
43	Surface Presentation of Functional Peptides in Solution Determines Cell Internalization Efficiency of TAT Conjugated Nanoparticles. Nano Letters, 2014, 14, 5229-5237.	4.5	44
44	Sulfur adsorption on Fe(110): a DFT study. Surface Science, 2003, 540, 420-430.	0.8	42
45	Density-functional theory studies of xanthate adsorption on the pyrite FeS2(110) and (111) surfaces. Journal of Chemical Physics, 2003, 118, 6022-6029.	1.2	42
46	A DFT study of the perovskite and hexagonal phases of BaTiO3. Computational Materials Science, 2005, 34, 157-165.	1.4	41
47	Molecular Simulation of Peptide Interactions with an RP-HPLC Sorbent. Journal of Physical Chemistry B, 1997, 101, 10962-10970.	1.2	40
48	Residue-Specific Solvation-Directed Thermodynamic and Kinetic Control over Peptide Self-Assembly with 1D/2D Structure Selection. ACS Nano, 2019, 13, 1900-1909.	7.3	40
49	Quantitative design rules for protein-resistant surface coatings using machine learning. Scientific Reports, 2019, 9, 265.	1.6	39
50	Cobalt-Directed Assembly of Antibodies onto Metalâ€“Phenolic Networks for Enhanced Particle Targeting. Nano Letters, 2020, 20, 2660-2666.	4.5	39
51	Effect of external stresses on protein conformation: a computer modelling study. European Biophysics Journal, 2004, 33, 121-129.	1.2	38
52	Adhesion between Graphite and Modified Polyester Surfaces:Â A Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 17224-17231.	1.2	38
53	Interaction of hydrogen with ZnO nanopowdersâ€”evidence of hydroxyl group formation. Nanotechnology, 2012, 23, 015705.	1.3	38
54	Comparative Study of Insulin Chain-B in Isolated and Monomeric Environments under External Stress. Journal of Physical Chemistry B, 2008, 112, 7916-7924.	1.2	37

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55	The structure of disordered carbon solids studied using a hybrid reverse Monte Carlo algorithm. Journal of Physics Condensed Matter, 2005, 17, 2605-2616.	0.7	36
56	Monolayer Structure and Evaporation Resistance: A Molecular Dynamics Study of Octadecanol on Water. Journal of Physical Chemistry B, 2010, 114, 3869-3878.	1.2	36
57	Facet-Dependent Interactions of Islet Amyloid Polypeptide with Gold Nanoparticles: Implications for Fibril Formation and Peptide-Induced Lipid Membrane Disruption. Chemistry of Materials, 2017, 29, 1550-1560.	3.2	35
58	First Principles Investigation of H Addition and Abstraction Reactions on Doped Aluminum Clusters. Journal of Physical Chemistry A, 2009, 113, 5832-5837.	1.1	34
59	Density functional theory modelling of and surfaces: Structure, properties and adsorption of N2O. Materials Chemistry and Physics, 2010, 119, 505-514.	2.0	34
60	DFT Study of H Adsorption on Magnesium-Doped Aluminum Clusters. Journal of Physical Chemistry A, 2010, 114, 3602-3608.	1.1	34
61	Metal-dependent inhibition of amyloid fibril formation: synergistic effects of cobaltâ€“tannic acid networks. Nanoscale, 2019, 11, 1921-1928.	2.8	34
62	H2S dissociation on the Fe(100) surface: An ab initio molecular dynamics study. Surface Science, 2008, 602, 1547-1553.	0.8	32
63	Layer-by-Layer Self-Assembly of Polymer Films and Capsules through Coiled-Coil Peptides. Chemistry of Materials, 2015, 27, 5820-5824.	3.2	32
64	Single-Step Homogeneous Immunoassays Utilizing Epitope-Tagged Gold Nanoparticles: On the Mechanism, Feasibility, and Limitations. Chemistry of Materials, 2014, 26, 4696-4704.	3.2	31
65	Effects of oxidation, pH and lipids on amyloidogenic peptide structure: implications for fibril formation?. European Biophysics Journal, 2008, 38, 99-110.	1.2	30
66	HRMC: Hybrid Reverse Monte Carlo method with silicon and carbon potentials. Computer Physics Communications, 2008, 178, 777-787.	3.0	30
67	Surface-water Interface Induces Conformational Changes Critical for Protein Adsorption: Implications for Monolayer Formation of EAS Hydrophobin. Frontiers in Molecular Biosciences, 2015, 2, 64.	1.6	29
68	â€œExactâ€•surface free energies of iron surfaces using a modified embedded atom method potential and Î» integration. Journal of Chemical Physics, 2004, 120, 3425-3430.	1.2	28
69	Identifying the Coiled-Coil Triple Helix Structure of Î²-Peptide Nanofibers at Atomic Resolution. ACS Nano, 2018, 12, 9101-9109.	7.3	28
70	Theoretical study of adhesion between graphite, polyester and silica surfaces. Molecular Simulation, 2005, 31, 449-455.	0.9	27
71	Simulations of Nanoindentation of Polymer Surfaces: Effects of Surface Cross-Linking on Adhesion and Hardness. Journal of Physical Chemistry C, 2010, 114, 478-486.	1.5	27
72	Surface heterogeneity: a friend or foe of protein adsorption â€“ insights from theoretical simulations. Faraday Discussions, 2016, 191, 435-464.	1.6	27

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73	High-performance liquid chromatography of amino acids, peptides and proteins. Journal of Chromatography A, 1994, 660, 75-84.	1.8	26
74	Coverage-Dependent Adsorption of Atomic Sulfur on Fe(110):Â A DFT Study. Journal of Physical Chemistry B, 2005, 109, 9604-9612.	1.2	25
75	Effects of Size and Functionalization on the Structure and Properties of Graphene Oxide Nanoflakes: An in Silico Investigation. ACS Omega, 2018, 3, 11497-11503.	1.6	25
76	Effects of forcefield and sampling method in all-atom simulations of inherently disordered proteins: Application to conformational preferences of human amylin. PLoS ONE, 2017, 12, e0186219.	1.1	25
77	Ab Initio Molecular Dynamics Study of H₂S Dissociation on the Fe(110) Surface. Journal of Physical Chemistry C, 2007, 111, 16372-16378.	1.5	24
78	An Active Site Inhibitor Induces Conformational Penalties for ACE2 Recognition by the Spike Protein of SARS-CoV-2. Journal of Physical Chemistry B, 2021, 125, 2533-2550.	1.2	24
79	Refinements in the collection of energy filtered diffraction patterns from disordered materials. Ultramicroscopy, 2005, 103, 275-283.	0.8	23
80	Classical Molecular Dynamics Study of [60]Fullerene Interactions with Silica and Polyester Surfaces. Journal of Physical Chemistry B, 2006, 110, 15963-15972.	1.2	23
81	Curved-Surface Atomic Modeling of Nanoporous Carbon. Journal of Physical Chemistry C, 2007, 111, 802-812.	1.5	23
82	Surface defects on ZnO nanowires: implications for design of sensors. Journal of Physics Condensed Matter, 2012, 24, 305001.	0.7	23
83	Molecular Mechanism of Stabilization of Thin Films for Improved Water Evaporation Protection. Langmuir, 2013, 29, 14451-14459.	1.6	23
84	Toward Cell Membrane Biomimetic Lipidic Cubic Phases: A High-Throughput Exploration of Lipid Compositional Space. ACS Applied Bio Materials, 2019, 2, 182-195.	2.3	23
85	Reactivity and Regioselectivity of Aluminum Nanoclusters: Insights from Regional Density Functional Theory. Journal of Physical Chemistry C, 2011, 115, 1714-1723.	1.5	22
86	Comparative Study of Commonly Used Molecular Dynamics Force Fields for Modeling Organic Monolayers on Water. Journal of Physical Chemistry B, 2011, 115, 3964-3971.	1.2	22
87	Gap Junction Hemichannel Interactions with Zwitterionic Lipid, Anionic Lipid, and Cholesterol: Molecular Simulation Studies. Biochemistry, 2011, 50, 1492-1504.	1.2	22
88	Fluorinated Metalâ€“Organic Coatings with Selective Wettability. Journal of the American Chemical Society, 2021, 143, 9972-9981.	6.6	21
89	On simulation methods to compute surface and interfacial free energies of disordered solids. Journal of Chemical Physics, 2002, 116, 8547.	1.2	20
90	Effect of S contamination on properties of Fe(100) surfaces. Surface Science, 2005, 590, 63-75.	0.8	20

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91	Nanoscale Wetting and Fouling Resistance of Functionalized Surfaces: A Computational Approach. Langmuir, 2014, 30, 10617-10625.	1.6	20
92	Universal simulation method to compute surface and interfacial free energies of disordered solids. Journal of Chemical Physics, 2002, 117, 7685-7690.	1.2	19
93	New lambda integration method to compute surface free energies of disordered surfaces. Journal of Chemical Physics, 2002, 117, 7676-7684.	1.2	19
94	Further studies of iron adhesion: () surfaces. Surface Science, 2002, 515, L464-L468.	0.8	19
95	Density-functional theory of xanthate adsorption on the pyrite FeS2(100) surface. Philosophical Magazine Letters, 2004, 84, 175-182.	0.5	19
96	Ab initio study of S dynamics on iron surfaces. Surface Science, 2007, 601, 665-671.	0.8	19
97	Effect of S Arrangement on Fe(110) Properties at 1/3 Monolayer Coverage:Â A DFT Study. Journal of Physical Chemistry B, 2006, 110, 956-962.	1.2	18
98	Molecular dynamics simulations of a fibrillogenic peptide derived from apolipoprotein C-II. Biophysical Chemistry, 2007, 130, 102-113.	1.5	18
99	Inhibition of peptide aggregation by lipids: Insights from coarse-grained molecular simulations. Journal of Molecular Graphics and Modelling, 2011, 29, 597-607.	1.3	18
100	Fate of Liposomes in the Presence of Phospholipase C and D: From Atomic to Supramolecular Lipid Arrangement. ACS Central Science, 2018, 4, 1023-1030.	5.3	18
101	Hydration and Dynamics of Ligands Determine the Antifouling Capacity of Functionalized Surfaces. Journal of Physical Chemistry C, 2019, 123, 30360-30372.	1.5	18
102	Siteâ€Selective Coordination Assembly of Dynamic Metalâ€Phenolic Networks. Angewandte Chemie - International Edition, 2022, 61, .	7.2	18
103	Effect of Surface Composition and Atomic Roughness on Interfacial Adhesion between Polyester and Amorphous Carbon. Journal of Physical Chemistry C, 2007, 111, 3000-3009.	1.5	17
104	Lipids Enhance Apolipoprotein C-II-Derived Amyloidogenic Peptide Oligomerization but Inhibit Fibril Formation. Journal of Physical Chemistry B, 2009, 113, 9447-9453.	1.2	17
105	Rational design of monolayers for improved water evaporation mitigation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 415, 47-58.	2.3	17
106	Exploring the binding sites and proton diffusion on insulin amyloid fibril surfaces by naphthol-based photoacid fluorescence and molecular simulations. Scientific Reports, 2017, 7, 6245.	1.6	17
107	A Cyclic Peptide Inhibitor of ApoC-II Peptide Fibril Formation: Mechanistic Insight from NMR and Molecular Dynamics Analysis. Journal of Molecular Biology, 2012, 416, 642-655.	2.0	16
108	Effect of Oxidation and Mutation on the Conformational Dynamics and Fibril Assembly of Amyloidogenic Peptides Derived from Apolipoprotein C-II. Journal of Physical Chemistry B, 2009, 113, 14006-14014.	1.2	15

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109	Effects of mutation on the amyloidogenic propensity of apolipoprotein C-II60â€“70 peptide. Physical Chemistry Chemical Physics, 2010, 12, 14762.	1.3	15
110	Hydrogen/Deuterium Exchange and Molecular Dynamics Analysis of Amyloid Fibrils Formed by a D69K Charge-Pair Mutant of Human Apolipoprotein C-II. Biochemistry, 2015, 54, 4805-4814.	1.2	15
111	Electromagnetic field modulates aggregation propensity of amyloid peptides. Journal of Chemical Physics, 2020, 152, 035104.	1.2	15
112	Prediction of liquid crystalline properties of poly(1,4-phenylene sebacate-oxybenzoate) by Monte Carlo simulation. Polymer, 2005, 46, 2003-2010.	1.8	14
113	Designing Fluorescent Peptide Sensors with Dual Specificity for the Detection of HIV-1 Protease. Chemistry of Materials, 2015, 27, 7187-7195.	3.2	14
114	Robust and Versatile Coatings Engineered via Simultaneous Covalent and Noncovalent Interactions. Angewandte Chemie - International Edition, 2021, 60, 20225-20230.	7.2	14
115	Characterization of Metallurgical Chars by Small Angle Neutron Scattering. Energy & Fuels, 2002, 16, 1009-1015.	2.5	13
116	Effect of Sulfur Impurity on Fe(110) Adhesion:Â A DFT Study. Journal of Physical Chemistry B, 2004, 108, 10965-10972.	1.2	13
117	Adsorption of atomic nitrogen and oxygen on mathrm {ZnO(2ar {1} ar {1}0)} surface: a density functional theory study. Journal of Physics Condensed Matter, 2009, 21, 144208.	0.7	13
118	"Janus" Cyclic Peptides: A New Approach to Amyloid Fibril Inhibition?. PLoS ONE, 2013, 8, e57437.	1.1	13
119	Three-Dimensional Organization of Self-Encapsulating Gluconobacter oxydans Bacterial Cells. ACS Omega, 2017, 2, 8099-8107.	1.6	13
120	Distinct Bimodal Roles of Aromatic Molecules in Controlling Gold Nanorod Growth for Biosensing. Advanced Functional Materials, 2017, 27, 1700523.	7.8	13
121	Monte Carlo based modeling of carbon nanostructured surfaces. Physical Review B, 2005, 72, .	1.1	12
122	Comb polymers: Are they the answer to monolayer stability?. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2011, 384, 482-489.	2.3	12
123	Molecular Interactions behind the Synergistic Effect in Mixed Monolayers of 1-Octadecanol and Ethylene Glycol Monooctadecyl Ether. Journal of Physical Chemistry B, 2013, 117, 3603-3612.	1.2	12
124	Lipid Concentration Effects on the Amyloidogenic apoC-II60â^'70 Peptide: A Computational Study. Journal of Physical Chemistry B, 2010, 114, 7974-7982.	1.2	11
125	Long-range dipolar order and dispersion forces in polar liquids. Journal of Chemical Physics, 2017, 147, 194503.	1.2	11
126	High-Throughput Peptide Derivatization toward Supramolecular Diversification in Microtiter Plates. ACS Nano, 2021, 15, 4034-4044.	7.3	11

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127	Origins of Structural Elasticity in Metalâ€“Phenolic Networks Probed by Super-Resolution Microscopy and Multiscale Simulations. ACS Nano, 2022, 16, 98-110.	7.3	11
128	Thermal behavior and molecular simulation of liquid crystalline polymers containing a pentamethylenic spacer. Computational Materials Science, 2003, 27, 393-402.	1.4	10
129	Molecular Dynamics Study of Polyester Surfaces and Fullerene Particles in Aqueous Environment. Journal of Physical Chemistry C, 2008, 112, 18141-18149.	1.5	10
130	Effect of Substrate on the Mechanical Response and Adhesion of PEGylated Surfaces: Insights from All-Atom Simulations. Langmuir, 2012, 28, 17263-17272.	1.6	10
131	Block Lengthâ€Dependent Protein Fouling on Poly(2â€oxazoline)â€Based Polymersomes: Influence on Macrophage Association and Circulation Behavior. Small, 2022, 18, .	5.2	10
132	Atomistic simulation of the sol formation during synthesis of organic/inorganic hybrid materials. Molecular Simulation, 2002, 28, 993-1004.	0.9	9
133	Molecular Simulation Study of Polymer Interactions with Silica Particles in Aqueous Solution. Journal of Physical Chemistry B, 2003, 107, 9681-9691.	1.2	9
134	Iron Surfaces: Pathways to Interfaces. Surface Review and Letters, 2003, 10, 169-174.	0.5	9
135	Surface crosslinking effects on contamination resistance of functionalised polymers. Soft Matter, 2013, 9, 1798-1806.	1.2	9
136	Response to Comment on â€œInfluence of the Chain Length and Surface Density on the Conformation and Mobility ofn-Alkyl Ligands Chemically Immobilized onto a Silica Surfaceâ€• Analytical Chemistry, 1996, 68, 1974-1975.	3.2	7
137	Effect of Sulfur Coverage on Fe(110) Adhesion:Â A DFT Study. Journal of Physical Chemistry B, 2005, 109, 10204-10212.	1.2	7
138	Effect of Aging on Interfacial Adhesion between Polyester and Carbon-Based Particles:â€‰ A Classical Molecular Dynamics Study. Journal of Physical Chemistry C, 2007, 111, 6465-6472.	1.5	7
139	Interaction of hydrogen with zinc oxide nanorods: why the spacing is important. Nanotechnology, 2011, 22, 135704.	1.3	7
140	Electromagnetic bioeffects: a multiscale molecular simulation perspective. Physical Chemistry Chemical Physics, 2022, 24, 6327-6348.	1.3	7
141	Density Functional Theory Study of Hydrogen Bonding in Ionic Molecular Materials. Journal of Physical Chemistry B, 2006, 110, 19605-19610.	1.2	6
142	Comparison of embedded atom method potentials for small aluminium cluster simulations. Journal of Physics Condensed Matter, 2009, 21, 144206.	0.7	6
143	Polymorphism in diseaseâ€related apolipoprotein Câ€II amyloid fibrils: a structural model for rodâ€like fibrils. FEBS Journal, 2018, 285, 2799-2812.	2.2	6
144	Nanoscale in silico classification of ligand functionalised surfaces for protein adsorption resistance. Nanoscale, 2020, 12, 7240-7255.	2.8	6

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145	Dynamic Performance of Duolayers at the Air/Water Interface. 2. Mechanistic Insights from All-Atom Simulations. Journal of Physical Chemistry B, 2014, 118, 10927-10933.	1.2	5
146	Solution Conditions Affect the Ability of the K30D Mutation To Prevent Amyloid Fibril Formation by Apolipoprotein C-II: Insights from Experiments and Theoretical Simulations. Biochemistry, 2016, 55, 3815-3824.	1.2	5
147	Intra- and Intersubunit Ion-Pair Interactions Determine the Ability of Apolipoprotein C-II Mutants To Form Hybrid Amyloid Fibrils. Biochemistry, 2017, 56, 1757-1767.	1.2	5
148	The Enigma of Amyloid Forming Proteins: Insights From Molecular Simulations. Australian Journal of Chemistry, 2019, 72, 574.	0.5	5
149	Hydrogen bonding in mixed ligand copper organophosphonates. Chemical Physics Letters, 2003, 378, 400-405.	1.2	4
150	Density Functional Theory Study of ZnO Nanostructures for NO and NO2 Sensing. , 2007, , .		4
151	Dynamic Performance of Duolayers at the Air/Water Interface. 1. Experimental Analysis. Journal of Physical Chemistry B, 2014, 118, 10919-10926.	1.2	4
152	Bioelectromagnetics Research within an Australian Context: The Australian Centre for Electromagnetic Bioeffects Research (ACEBR). International Journal of Environmental Research and Public Health, 2016, 13, 967.	1.2	4
153	Gold Nanoparticles: Understanding and Designing the Gold-Bio Interface: Insights from Simulations (Small 18/2016). Small, 2016, 12, 2394-2394.	5.2	4
154	Effect of substrate on the responsive behaviour of functionalised surfaces: insights from molecular simulation. Molecular Simulation, 2016, 42, 563-572.	0.9	4
155	Design of Lipid-Based Nanocarriers via Cation Modulation of Ethanol-Interdigitated Lipid Membranes. Langmuir, 2021, 37, 11909-11921.	1.6	4
156	Effect of Water Concentration on Sol Formation in Synthesis of Organic/Inorganic Hybrid Materials. Molecular Simulation, 2003, 29, 231-233.	0.9	3
157	Regional DFTâ€"Electronic Stress Tensor Study of Aluminum Nanostructures for Hydrogen Storage. , 2009, , .		3
158	Molecular modelling of peptide folding, misfolding and aggregation phenomena. Procedia Computer Science, 2010, 1, 1185-1193.	1.2	3
159	Role of Hydrogen in Dimerizaton of Aluminum Clusters: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 7734-7743.	1.1	3
160	HRMC_1.1: Hybrid Reverse Monte Carlo method with silicon and carbon potentials. Computer Physics Communications, 2011, 182, 542.	3.0	3
161	Translocation of silica nanospheres through giant unilamellar vesicles (GUVs) induced by a high frequency electromagnetic field. RSC Advances, 2021, 11, 31408-31420.	1.7	3
162	Quantum Monte Carlo Study of Water Molecule: A Preliminary Investigation. Australian Journal of Chemistry, 2004, 57, 1229.	0.5	3

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163	Siteâ€Selective Coordination Assembly of Dynamic Metalâ€“Phenolic Networks. Angewandte Chemie, 0, , .	1.6	3
164	A molecular dynamics study of siloxane diffusion in a polyesterâ€“melamine solution. Polymer, 2007, 48, 2179-2185.	1.8	2
165	Effects of graphitic nanomaterials on the dissociation pathway of amyloidogenic peptide dimer. , 2014, , .		2
166	Robust and Versatile Coatings Engineered via Simultaneous Covalent and Noncovalent Interactions. Angewandte Chemie, 2021, 133, 20387-20392.	1.6	2
167	Insights On Protein Structure And Dynamics From Multiple Biased Molecular Dynamics Simulations. Biophysical Journal, 2009, 96, 589a.	0.2	0
168	Molecular rationale for the structure of cyclic poly(methyl methacrylate) stereocomplexes. , 2014, , .		0
169	Applications: general discussion. Faraday Discussions, 2016, 191, 565-595.	1.6	0