Susanna Monti

List of Publications by Year
in descending order

123 papers	3,272 citations	136950 32 h-index	182427 51 g-index
126 all docs	126 docs citations	126 times ranked	3763 citing authors

#	Article	IF	Citations
1	Electronic Energy Transfer in Condensed Phase Studied by a Polarizable QM/MM Model. Journal of Chemical Theory and Computation, 2009, 5, 1838-1848.	5.3	259
2	Novel imidazole-based combretastatin A-4 analogues: Evaluation of their in vitro antitumor activity and molecular modeling study of their binding to the colchicine site of tubulin. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 5757-5762.	2.2	112
3	Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field. Physical Chemistry Chemical Physics, 2013, 15, 15062.	2.8	111
4	Peptideâ^'TiO2Surface Interaction in Solution by Ab Initio and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 6160-6169.	2.6	109
5	Dispersion corrected DFT approaches for anharmonic vibrational frequency calculations: nucleobases and their dimers. Physical Chemistry Chemical Physics, 2014, 16, 10112-10128.	2.8	92
6	Joyce and Ulysses: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data. Physical Chemistry Chemical Physics, 2013, 15, 3736.	2.8	89
7	Exploration of the Conformational and Reactive Dynamics of Glycine and Diglycine on TiO₂: Computational Investigations in the Gas Phase and in Solution. Journal of Physical Chemistry C, 2012, 116, 5141-5150.	3.1	83
8	Lignin-Supported Heterogeneous Photocatalyst for the Direct Generation of H₂O₂ from Seawater. Journal of the American Chemical Society, 2022, 144, 2603-2613.	13.7	80
9	Absorption and Emission Spectra of a Flexible Dye in Solution: A Computational Time-Dependent Approach. Journal of Chemical Theory and Computation, 2013, 9, 4507-4516.	5.3	78
10	Environmental Effects on the Spectroscopic Properties of Gallic Acid:â€‰ A Combined Classical and Quantum Mechanical Study. Journal of Physical Chemistry A, 2005, 109, 1933-1943.	2.5	71
11	Absorption and emission UV-Vis spectra of the TRITC fluorophore molecule in solution: a quantum mechanical study. Physical Chemistry Chemical Physics, 2010, 12, 1000-1006.	2.8	67
12	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	64
13	Interaction of Î²-Sheet Folds with a Gold Surface. PLoS ONE, 2011, 6, e20925.	2.5	61
14	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. Physical Chemistry Chemical Physics, 2011, 13, 2160-2166.	2.8	57
15	Realistic Modeling of Fluorescent Dye-Doped Silica Nanoparticles: A Step Toward the Understanding of their Enhanced Photophysical Properties.. Chemistry of Materials, 2011, 23, 5016-5023.	6.7	57
16	Reactive Dynamics Simulation of Monolayer and Multilayer Adsorption of Glycine on Cu(110). Journal of Physical Chemistry C, 2013, 117, 5221-5228.	3.1	54
17	On the Calculation of Vibrational Frequencies for Molecules in Solution Beyond the Harmonic Approximation. Journal of Chemical Theory and Computation, 2010, 6, 1660-1669.	5.3	52
18	Towards the design of highly selective recognition sites into molecular imprinting polymers: A computational approach. Biosensors and Bioelectronics, 2006, 22, 153-163.	10.1	49

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19	Cellulose Nanofiberâ€“Graphene Oxide Biohybrids: Disclosing the Self-Assembly and Copper-Ion Adsorption Using Advanced Microscopy and ReaxFF Simulations. ACS Nano, 2018, 12, 7028-7038.	14.6	46
20	Computational Study of the One- and Two-Photon Absorption and Circular Dichroism of (<scp>l</scp>)-Tryptophan. Journal of Physical Chemistry B, 2010, 114, 6500-6512.	2.6	45
21	Molecular Dynamics Simulations of Collagen-like Peptide Adsorption on Titanium-Based Material Surfaces. Journal of Physical Chemistry C, 2007, 111, 6086-6094.	3.1	44
22	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. Physical Chemistry Chemical Physics, 2010, 12, 10550.	2.8	43
23	Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 272-276.	4.6	43
24	Adsorption of Ionic Peptides on Inorganic Supports. Journal of Physical Chemistry C, 2009, 113, 2433-2442.	3.1	41
25	Understanding the Structural and Binding Properties of Collagen:â€‰ A Theoretical Perspective. Journal of Physical Chemistry B, 2004, 108, 10101-10112.	2.6	39
26	Effects Due to Interadsorbate Interactions on the Dipeptide/TiO2Surface Binding Mechanism Investigated by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2007, 111, 7765-7771.	3.1	38
27	Absorption and emission spectra of fluorescent silica nanoparticles from TD-DFT/MM/PCM calculations. Physical Chemistry Chemical Physics, 2011, 13, 16689.	2.8	36
28	Simulations of Lipid Adsorption on TiO₂ Surfaces in Solution. Langmuir, 2008, 24, 10145-10154.	3.5	35
29	Journey toward the Surface: How Glycine Adsorbs on Titania in Water Solution. Journal of Physical Chemistry C, 2012, 116, 18318-18326.	3.1	34
30	Characterization of the adsorption dynamics of trisodium citrate on gold in water solution. RSC Advances, 2017, 7, 49655-49663.	3.6	33
31	Nanocellulose/graphene oxide layered membranes: elucidating their behaviour during filtration of water and metal ions in real time. Nanoscale, 2019, 11, 22413-22422.	5.6	33
32	Atomic-Level Understanding for the Enhanced Generation of Hydrogen Peroxide by the Introduction of an Aryl Amino Group in Polymeric Carbon Nitrides. ACS Catalysis, 2021, 11, 14087-14101.	11.2	33
33	An Integrated Protocol for the Accurate Calculation of Magnetic Interactions in Organic Magnets. Journal of Chemical Theory and Computation, 2011, 7, 699-706.	5.3	32
34	Structure and dynamics of gold nanoparticles decorated with chitosanâ€“gentamicin conjugates: ReaxFF molecular dynamics simulations to disclose drug delivery. Physical Chemistry Chemical Physics, 2019, 21, 13099-13108.	2.8	32
35	New Mechanistic Insights into the Lignin Î²-O-4 Linkage Acidolysis with Ethylene Glycol Stabilization Aided by Multilevel Computational Chemistry. ACS Sustainable Chemistry and Engineering, 2021, 9, 2388-2399.	6.7	32
36	Quantum molecular dynamics study of water on TiO2(110) surface. Journal of Chemical Physics, 2008, 129, 064703.	3.0	30

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37	Dynamics and self-assembly of bio-functionalized gold nanoparticles in solution: Reactive molecular dynamics simulations. Nano Research, 2018, 11, 1757-1767.	10.4	29
38	Toward the Supramolecular Structure of Collagen:Â A Molecular Dynamics Approach. Journal of Physical Chemistry B, 2005, 109, 11389-11398.	2.6	28
39	Multivalent ion-induced re-entrant transition of carboxylated cellulose nanofibrils and its influence on nanomaterialsâ€™ properties. Nanoscale, 2020, 12, 15652-15662.	5.6	28
40	Effect of the environment on vibrational infrared and circular dichroism spectra of (s)-proline. International Journal of Quantum Chemistry, 2005, 104, 744-757.	2.0	26
41	RAD16II Î²-Sheet Filaments onto Titanium Dioxide:â€‰ Dynamics and Adsorption Properties. Journal of Physical Chemistry C, 2007, 111, 16962-16973.	3.1	26
42	Decoration of gold nanoparticles with cysteine in solution: reactive molecular dynamics simulations. Nanoscale, 2016, 8, 12929-12938.	5.6	26
43	Magnetic Interactions in Phenyl-Bridged Nitroxide Diradicals: Conformational Effects by Multireference and Broken Symmetry DFT Approaches. Journal of Physical Chemistry A, 2009, 113, 15150-15155.	2.5	25
44	Structureâ€“Properties Relationships in Triplet Ground State Organic Diradicals: A Computational Study. Journal of Chemical Theory and Computation, 2013, 9, 300-307.	5.3	24
45	Evaluation of nanocellulose interaction with water pollutants using nanocellulose colloidal probes and molecular dynamic simulations. Carbohydrate Polymers, 2020, 229, 115510.	10.2	24
46	Conformations of Phenylalanine in the Tripeptides AFA and GFG Probed by Combining MD Simulations with NMR, FTIR, Polarized Raman, and VCD Spectroscopy. Journal of Physical Chemistry B, 2010, 114, 3965-3978.	2.6	23
47	The effects of ferulic acid on Î²-amyloid fibrillar structures investigated through experimental and computational techniques. Biochimica Et Biophysica Acta - General Subjects, 2013, 1830, 2924-2937.	2.4	23
48	Theoretical Investigation of Adsorption, Dynamics, Self-Aggregation, and Spectroscopic Properties of the D102 Indoline Dye on an Anatase (101) Substrate. Journal of Physical Chemistry C, 2016, 120, 2787-2796.	3.1	23
49	Molecular dynamics simulations of melting and sintering of Si nanoparticles: a comparison of different force fields and computational models. Physical Chemistry Chemical Physics, 2018, 20, 1707-1715.	2.8	23
50	NEXAFS and XPS studies of nitrosyl chloride. Physical Chemistry Chemical Physics, 2015, 17, 9040-9048.	2.8	22
51	Toward Sustainable Li-Ion Battery Recycling: Green Metalâ€“Organic Framework as a Molecular Sieve for the Selective Separation of Cobalt and Nickel. ACS Sustainable Chemistry and Engineering, 2021, 9, 9770-9778.	6.7	22
52	Molecular Dynamics Simulations of the Adsorption and Dynamical Behavior of Single DNA Components on TiO₂. Journal of Physical Chemistry C, 2011, 115, 24238-24246.	3.1	21
53	Computational study of conformational and chiroptical properties of (2R,3S,4R)-(+)-3,3â€²,4,4â€²,7-flavanpentol. Chirality, 2005, 17, 577-589.	2.6	20
54	Singletâ€“triplet energy gap of a diarylnitroxide diradical by an accurate many-body perturbative approach. Physical Chemistry Chemical Physics, 2011, 13, 4709.	2.8	19

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55	Molecular Dynamics Simulations of the Self-Assembly of Tetraphenylporphyrin-Based Monolayers and Bilayers at a Silver Interface. Journal of Physical Chemistry C, 2011, 115, 18434-18444.	3.1	18
56	5-fluorouracil dimers in aqueous solution: molecular dynamics in water and continuum solvation. International Journal of Quantum Chemistry, 2002, 88, 133-146.	2.0	17
57	Sensors for DNA detection: theoretical investigation of the conformational properties of immobilized single-strand DNA. Physical Chemistry Chemical Physics, 2009, 11, 10644.	2.8	16
58	Cysteine on TiO₂(110): A Theoretical Study by Reactive Dynamics and Photoemission Spectra Simulation. Langmuir, 2014, 30, 8819-8828.	3.5	16
59	Dropping a Droplet of Cysteine Molecules on a Rutile (110) Interface: Reactive versus Nonreactive Classical Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 6703-6712.	3.1	16
60	Experimental and theoretical XPS and NEXAFS studies of N-methylacetamide and N-methyltrifluoroacetamide. Physical Chemistry Chemical Physics, 2016, 18, 2210-2218.	2.8	16
61	Parametrization of a Reactive Force Field (ReaxFF) for Molecular Dynamics Simulations of Si Nanoparticles. Journal of Chemical Theory and Computation, 2017, 13, 3854-3861.	5.3	16
62	ReaxFF Simulations of Lignin Fragmentation on a Palladium-Based Heterogeneous Catalyst in Methanolâ€“Water Solution. Journal of Physical Chemistry Letters, 2018, 9, 5233-5239.	4.6	16
63	Theoretical investigation of histidine-tryptophan preferential interactions. Theoretical Chemistry Accounts, 1999, 101, 143-150.	1.4	15
64	Interaction of collagen with chlorosulphonated paraffin tanning agents: Fourier transform infrared spectroscopic analysis and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 14736.	2.8	15
65	Hybrid density functionalâ€“molecular mechanics calculations for core-electron binding energies of glycine in water solution. Physical Chemistry Chemical Physics, 2013, 15, 244-254.	2.8	15
66	Synthesis of biphenylyltetrazole derivatives of 1-aminopyrroles as angiotensin II antagonists. Il Farmaco, 1999, 54, 64-76.	0.9	14
67	Adsorption of Collagen Nanofibrils on Rough TiO₂: A Molecular Dynamics Study. Advanced Engineering Materials, 2011, 13, B334.	3.5	14
68	1,2-Disubstituted cyclohexane derived tripeptide aldehydes as novel selective thrombin inhibitors. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 1249-1254.	2.2	13
69	B3LYP/6-31G* conformational landscape in vacuo of some pterocarpan stereoisomers with biological activity. Physical Chemistry Chemical Physics, 2004, 6, 2849.	2.8	13
70	Interaction of biomolecular systems with titanium-based materials: computational investigations. Theoretical Chemistry Accounts, 2009, 123, 299-309.	1.4	13
71	Simulating DNA Hybridization on an Amine-Functionalized Silicon Substrate. Journal of Physical Chemistry B, 2010, 114, 8341-8349.	2.6	13
72	Surface-Altered Protonation Studied by Photoelectron Spectroscopy and Reactive Dynamics Simulations. Journal of Physical Chemistry Letters, 2015, 6, 807-811.	4.6	13

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73	Design of ultrathin hybrid membranes with improved retention efficiency of molecular dyes. RSC Advances, 2019, 9, 28657-28669.	3.6	13
74	Continuum solvent effects on various isomers of bilirubin. Physical Chemistry Chemical Physics, 2000, 2, 4884-4890.	2.8	12
75	Molecular dynamics and Monte Carlo simulations for the structure of the aqueous trimethylammonium chloride solution in the 0.2â€“1 molar range. Physical Chemistry Chemical Physics, 2011, 13, 6270.	2.8	12
76	Theoretical Study of the Adsorption Mechanism of Cystine on Au(110) in Aqueous Solution. Small, 2016, 12, 6134-6143.	10.0	12
77	Ab initio modeling of competitive drug-drug interactions: 5-fluorouracil dimers in the gas phase and in solution. International Journal of Quantum Chemistry, 2001, 83, 128-142.	2.0	11
78	Parameterization and validation of an accurate force-field for the simulation of alkylamine functionalized silicon (111) surfaces. Physical Chemistry Chemical Physics, 2010, 12, 4201.	2.8	11
79	Interactions of Nucleotide Bases with Decorated Si Surfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2011, 115, 9146-9156.	3.1	11
80	Theoretical Simulations of Structure and X-ray Photoelectron Spectra of Glycine and Diglycine Adsorbed on Cu(110). Langmuir, 2013, 29, 10194-10204.	3.5	11
81	Computational Study of Acidic and Basic Functionalized Crystalline Silica Surfaces as a Model for Biomaterial Interfaces. Langmuir, 2015, 31, 6321-6331.	3.5	11
82	Structure and Dynamics of the Hydrogen-Bond Network around (R,R)-Pterocarpans with Biological Activity in Aqueous Solution. Journal of Physical Chemistry B, 2005, 109, 16918-16925.	2.6	10
83	Characterization of Supramolecular Polyphenolâ^'Chromium(III) Clusters by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 13227-13234.	2.6	10
84	Diverse Phases of Carbonaceous Materials from Stochastic Simulations. ACS Nano, 2021, 15, 6369-6385.	14.6	10
85	Conformational Analysis of Glyâ€“Alaâ€“NHMe in D₂O and DMSO Solutions: A Two-Dimensional Infrared Spectroscopy Study. Journal of Physical Chemistry B, 2013, 117, 14226-14237.	2.6	9
86	A Computational Study of the Adsorption and Reactive Dynamics of Diglycine on Cu(110). Journal of Physical Chemistry C, 2014, 118, 3610-3619.	3.1	9
87	Optical Properties of Gold Nanoclusters Functionalized with a Small Organic Compound: Modeling by an Integrated Quantum-Classical Approach. Journal of Chemical Theory and Computation, 2016, 12, 3325-3339.	5.3	9
88	Modeling Nucleation and Growth of ZnO Nanoparticles in a Low Temperature Plasma by Reactive Dynamics. Journal of Chemical Theory and Computation, 2019, 15, 2010-2021.	5.3	9
89	Enhanced sieving of cellulosic microfiber membranesviatuning of interlayer spacing. Environmental Science: Nano, 2020, 7, 2941-2952.	4.3	9
90	A combination of experimental and computational methods to study the reactions during a Lignin-First approach. Pure and Applied Chemistry, 2020, 92, 631-639.	1.9	9

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91	Microscopic Hybrid Membranes Made of Cellulose-Based Materials Tuned for Removing Metal Ions from Industrial Effluents. ACS Applied Polymer Materials, 2021, 3, 3733-3746.	4.4	9
92	Conformation and Orientation of Tetraalanine in a Lyotropic Liquid Crystal Studied by Nuclear Magnetic Resonance. Journal of Physical Chemistry B, 2005, 109, 21102-21109.	2.6	8
93	Ionic Peptide Aggregation:Â Exploration of Conformational Dynamics in Aqueous Solution by Computational Techniques. Journal of Physical Chemistry B, 2007, 111, 1165-1175.	2.6	8
94	Hydration of cyanin dyes. Journal of Chemical Physics, 2010, 132, 114304.	3.0	8
95	Experimental and theoretical elucidation of catalytic pathways in TiO₂-initiated prebiotic polymerization. Physical Chemistry Chemical Physics, 2019, 21, 5435-5447.	2.8	8
96	Interaction of a Tripeptide with Cesium Perfluorooctanoate Micelles. Journal of Physical Chemistry B, 2008, 112, 1251-1261.	2.6	7
97	Influence of structural features on the selfâ€assembly of short ionic oligopeptides. Journal of Polymer Science Part A, 2010, 48, 889-897.	2.3	7
98	DNA hybridization mechanism on silicon nanowires: a molecular dynamics approach. Molecular BioSystems, 2010, 6, 2230.	2.9	7
99	Theoretical study of the conformational and optical properties of a fluorescent dye. A step toward modeling sensors grafted on polymer structures. Physical Chemistry Chemical Physics, 2011, 13, 21471.	2.8	7
100	Evidences of long lived cages in functionalized polymers: Effects on chromophore dynamic and spectroscopic properties. Chemical Physics Letters, 2014, 601, 134-138.	2.6	7
101	Atomistic Modelling of Si Nanoparticles Synthesis. Crystals, 2017, 7, 54.	2.2	7
102	Optimization of a New Reactive Force Field for Silver-Based Materials. Journal of Chemical Theory and Computation, 2020, 16, 7089-7099.	5.3	7
103	On the mineralization of nanocellulose to produce functional hybrid materials. Journal of Materials Chemistry A, 2022, 10, 9248-9276.	10.3	7
104	Upscaled engineered functional microfibrillated cellulose flat sheet membranes for removing charged water pollutants. Separation and Purification Technology, 2022, 289, 120745.	7.9	7
105	Cholic Acid Derivatives Containing Both 2-Naphthylcarbamate and 3,5-Dinitrophenylcarbamate Groups:Â A Combined Circular Dichroismâ^Molecular Mechanics Approach to the Definition of Their Molecular Conformation. Journal of Organic Chemistry, 2003, 68, 3145-3157.	3.2	6
106	Partially folded states of HIV-1 protease: Molecular dynamics simulations and ligand binding. Computational and Theoretical Chemistry, 2006, 769, 111-121.	1.5	6
107	Organic Functionalization and Optimal Coverage of a Silicon(111) Surface in Solvent: A Computational Study. Journal of Physical Chemistry C, 2011, 115, 4145-4154.	3.1	6
108	Modeling generation and growth of iron oxide nanoparticles from representative precursors through ReaxFF molecular dynamics. Nanoscale, 2020, 12, 3103-3111.	5.6	6

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109	Thermal degradation of optical resonances in plasmonic nanoparticles. Nanoscale, 2022, 14, 433-447.	5.6	6
110	Reaction pathways on N-substituted carbon catalysts during the electrochemical reduction of nitrate to ammonia. Catalysis Science and Technology, 2022, 12, 3582-3593.	4.1	6
111	Theoretical study of para-nitro-aniline adsorption on the Au(111) surface. Surface Science, 2016, 649, 124-132.	1.9	5
112	A close view of the organic linker in a MOF: structural insights from a combined ¹H NMR relaxometry and computational investigation. Physical Chemistry Chemical Physics, 2020, 22, 15222-15230.	2.8	5
113	Complementary and partially complementary DNA duplexes tethered to a functionalized substrate: a molecular dynamics approach to biosensing. Physical Chemistry Chemical Physics, 2011, 13, 12478.	2.8	4
114	Structure and Dynamics of Perylene Bisimide Pigments for â€œCoolâ€•Organic Coatings by Solid-State NMR: A Combined Experimental and DFT Study. Journal of Physical Chemistry C, 2020, 124, 17971-17980.	3.1	4
115	Dynamical and Structural Characterization of the Adsorption of Fluorinated Alkane Chains onto CeO₂. Journal of Physical Chemistry C, 2018, 122, 23405-23413.	3.1	3
116	pH-dependent X-ray Photoelectron Chemical Shifts and Surface Distribution of Cysteine in Aqueous Solution. Journal of Physical Chemistry B, 2019, 123, 3776-3785.	2.6	3
117	A test case for time-dependent density functional theory calculations of electronic circular dichroism: 2-chloro-4-methoxy-6- [(R)-1-phenylethylamino]-1,3,5- triazine. Theoretical Chemistry Accounts, 2007, 117, 793-803.	1.4	1
118	Study of the Interaction of GFG Tripeptide with Cesium Perfluorooctanoate Micelles by Means of NMR Spectroscopy and MD Simulations. Langmuir, 2008, 24, 5809-5815.	3.5	1
119	Reactive force field simulations of silicon clusters. Advances in Physics: X, 2019, 4, 1634487.	4.1	1
120	Correction to â€œNew Mechanistic Insights into the Lignin Î²-O-4 Linkage Acidolysis with Ethylene Glycol Stabilization Aided by Multilevel Computational Chemistryâ€• ACS Sustainable Chemistry and Engineering, 2021, 9, 9149-9149.	6.7	1
121	Chemo-enzymatic functionalized sustainable cellulosic membranes: Impact of regional selectivity on ions capture and antifouling behavior. Carbohydrate Polymers, 2022, 278, 118937.	10.2	1
122	Hybrid Materials: Theoretical Study of the Adsorption Mechanism of Cystine on Au(110) in Aqueous Solution (Small 44/2016). Small, 2016, 12, 6046-6046.	10.0	0
123	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Highlights in Theoretical Chemistry, 2013, , 319-337.	0.0	0