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	Chemo-enzymatic functionalized sustainable cellulosic membranes: Impact of regional selectivity on ions capture and antifouling behavior. Carbohydrate Polymers, 2022, 278, 118937.	10.2	1
2	Thermal degradation of optical resonances in plasmonic nanoparticles. Nanoscale, 2022, 14, 433-447.	5.6	6
3	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
4	On the mineralization of nanocellulose to produce functional hybrid materials. Journal of Materials Chemistry A, 2022, 10, 9248-9276.	10.3	7
5	Upscaled engineered functional microfibrillated cellulose flat sheet membranes for removing charged water pollutants. Separation and Purification Technology, 2022, 289, 120745.	7.9	7
6	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
7	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
8	Diverse Phases of Carbonaceous Materials from Stochastic Simulations. ACS Nano, 2021, 15, 6369-6385.	14.6	10
9	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
10	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
11	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
12	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
13	Evaluation of nanocellulose interaction with water pollutants using nanocellulose colloidal probes and molecular dynamic simulations. Carbohydrate Polymers, 2020, 229, 115510.	10.2	24
14	Modeling generation and growth of iron oxide nanoparticles from representative precursors through ReaxFF molecular dynamics. Nanoscale, 2020, 12, 3103-3111.	5.6	6
15	Optimization of a New Reactive Force Field for Silver-Based Materials. Journal of Chemical Theory and Computation, 2020, 16, 7089-7099.	5.3	7
16	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
17	Enhanced sieving of cellulosic microfiber membranesviatuning of interlayer spacing. Environmental Science: Nano, 2020, 7, 2941-2952.	4.3	9
18	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

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19	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
20	Multivalent ion-induced re-entrant transition of carboxylated cellulose nanofibrils and its influence on nanomaterialsâ€™ properties. Nanoscale, 2020, 12, 15652-15662.	5.6	28
21	Reactive force field simulations of silicon clusters. Advances in Physics: X, 2019, 4, 1634487.	4.1	1
22	Design of ultrathin hybrid membranes with improved retention efficiency of molecular dyes. RSC Advances, 2019, 9, 28657-28669.	3.6	13
23	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
24	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
25	Experimental and theoretical elucidation of catalytic pathways in TiO₂-initiated prebiotic polymerization. Physical Chemistry Chemical Physics, 2019, 21, 5435-5447.	2.8	8
26	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
27	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
28	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
29	Dynamics and self-assembly of bio-functionalized gold nanoparticles in solution: Reactive molecular dynamics simulations. Nano Research, 2018, 11, 1757-1767.	10.4	29
30	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
31	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
32	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
33	Characterization of the adsorption dynamics of trisodium citrate on gold in water solution. RSC Advances, 2017, 7, 49655-49663.	3.6	33
34	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
35	Atomistic Modelling of Si Nanoparticles Synthesis. Crystals, 2017, 7, 54.	2.2	7
36	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

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37	Theoretical Study of the Adsorption Mechanism of Cystine on Au(110) in Aqueous Solution. Small, 2016, 12, 6134-6143.	10.0	12
38	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
39	Decoration of gold nanoparticles with cysteine in solution: reactive molecular dynamics simulations. Nanoscale, 2016, 8, 12929-12938.	5.6	26
40	Theoretical study of para-nitro-aniline adsorption on the Au(111) surface. Surface Science, 2016, 649, 124-132.	1.9	5
41	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
42	Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 272-276.	4.6	43
43	Experimental and theoretical XPS and NEXAFS studies of N-methylacetamide and N-methyltrifluoroacetamide. Physical Chemistry Chemical Physics, 2016, 18, 2210-2218.	2.8	16
44	Surface-Altered Protonation Studied by Photoelectron Spectroscopy and Reactive Dynamics Simulations. Journal of Physical Chemistry Letters, 2015, 6, 807-811.	4.6	13
45	NEXAFS and XPS studies of nitrosyl chloride. Physical Chemistry Chemical Physics, 2015, 17, 9040-9048.	2.8	22
46	Computational Study of Acidic and Basic Functionalized Crystalline Silica Surfaces as a Model for Biomaterial Interfaces. Langmuir, 2015, 31, 6321-6331.	3.5	11
47	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
48	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
49	Dispersion corrected DFT approaches for anharmonic vibrational frequency calculations: nucleobases and their dimers. Physical Chemistry Chemical Physics, 2014, 16, 10112-10128.	2.8	92
50	Cysteine on TiO₂(110): A Theoretical Study by Reactive Dynamics and Photoemission Spectra Simulation. Langmuir, 2014, 30, 8819-8828.	3.5	16
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	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
63	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
64	Journey toward the Surface: How Glycine Adsorbs on Titania in Water Solution. Journal of Physical Chemistry C, 2012, 116, 18318-18326.	3.1	34
65	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
66	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
67	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
68	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
69	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
70	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
71	Interactions of Nucleotide Bases with Decorated Si Surfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2011, 115, 9146-9156.	3.1	11
72	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

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73	Absorption and emission spectra of fluorescent silica nanoparticles from TD-DFT/MM/PCM calculations. Physical Chemistry Chemical Physics, 2011, 13, 16689.	2.8	36
74	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. Physical Chemistry Chemical Physics, 2011, 13, 2160-2166.	2.8	57
75	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
76	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
77	Interaction of Î²-Sheet Folds with a Gold Surface. PLoS ONE, 2011, 6, e20925.	2.5	61
78	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
79	Adsorption of Collagen Nanofibrils on Rough TiO₂: A Molecular Dynamics Study. Advanced Engineering Materials, 2011, 13, B334.	3.5	14
80	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
81	Hydration of cyanin dyes. Journal of Chemical Physics, 2010, 132, 114304.	3.0	8
82	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
83	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
84	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
85	Simulating DNA Hybridization on an Amine-Functionalized Silicon Substrate. Journal of Physical Chemistry B, 2010, 114, 8341-8349.	2.6	13
86	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
87	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. Physical Chemistry Chemical Physics, 2010, 12, 10550.	2.8	43
88	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
89	DNA hybridization mechanism on silicon nanowires: a molecular dynamics approach. Molecular BioSystems, 2010, 6, 2230.	2.9	7
90	Interaction of biomolecular systems with titanium-based materials: computational investigations. Theoretical Chemistry Accounts, 2009, 123, 299-309.	1.4	13

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91	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
92	Adsorption of Ionic Peptides on Inorganic Supports. Journal of Physical Chemistry C, 2009, 113, 2433-2442.	3.1	41
93	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
94	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
95	Interaction of a Tripeptide with Cesium Perfluorooctanoate Micelles. Journal of Physical Chemistry B, 2008, 112, 1251-1261.	2.6	7
96	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
97	Simulations of Lipid Adsorption on TiO₂ Surfaces in Solution. Langmuir, 2008, 24, 10145-10154.	3.5	35
98	Quantum molecular dynamics study of water on TiO2(110) surface. Journal of Chemical Physics, 2008, 129, 064703.	3.0	30
99	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
100	RAD16II Î²-Sheet Filaments onto Titanium Dioxide:â€‰ Dynamics and Adsorption Properties. Journal of Physical Chemistry C, 2007, 111, 16962-16973.	3.1	26
101	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
102	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
103	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
104	Characterization of Supramolecular Polyphenolâ^'Chromium(III) Clusters by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 13227-13234.	2.6	10
105	Peptideâ^'TiO2Surface Interaction in Solution by Ab Initio and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 6160-6169.	2.6	109
106	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
107	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
108	Partially folded states of HIV-1 protease: Molecular dynamics simulations and ligand binding. Computational and Theoretical Chemistry, 2006, 769, 111-121.	1.5	6

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109	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
110	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
111	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
112	Toward the Supramolecular Structure of Collagen:Â A Molecular Dynamics Approach. Journal of Physical Chemistry B, 2005, 109, 11389-11398.	2.6	28
113	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
114	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
115	B3LYP/6-31G* conformational landscape in vacuo of some pterocarpan stereoisomers with biological activity. Physical Chemistry Chemical Physics, 2004, 6, 2849.	2.8	13
116	Understanding the Structural and Binding Properties of Collagen:â€‰ A Theoretical Perspective. Journal of Physical Chemistry B, 2004, 108, 10101-10112.	2.6	39
117	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
118	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
119	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
120	Continuum solvent effects on various isomers of bilirubin. Physical Chemistry Chemical Physics, 2000, 2, 4884-4890.	2.8	12
121	Theoretical investigation of histidine-tryptophan preferential interactions. Theoretical Chemistry Accounts, 1999, 101, 143-150.	1.4	15
122	Synthesis of biphenylyltetrazole derivatives of 1-aminopyrroles as angiotensin II antagonists. Il Farmaco, 1999, 54, 64-76.	0.9	14
123	1,2-Disubstituted cyclohexane derived tripeptide aldehydes as novel selective thrombin inhibitors. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 1249-1254.	2.2	13