Marco Pagliai

List of Publications by Year
in descending order

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91 papers	2,282 citations	236925 25 h-index	254184 43 g-index
91 all docs	91 docs citations	91 times ranked	2957 citing authors

#	Article	IF	Citations
1	Hydrogen bond dynamics in liquid methanol. Journal of Chemical Physics, 2003, 119, 6655-6662.	3.0	171
2	Identification of potential binders of the main protease 3CLpro of the COVID-19 via structure-based ligand design and molecular modeling. Chemical Physics Letters, 2020, 750, 137489.	2.6	133
3	Assessment of GAFF2 and OPLS-AA General Force Fields in Combination with the Water Models TIP3P, SPCE, and OPC3 for the Solvation Free Energy of Druglike Organic Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1983-1995.	5.3	131
4	The Vibrational Spectrum of Fullerene C60. Journal of Physical Chemistry A, 2001, 105, 11192-11196.	2.5	126
5	SERS, XPS, and DFT Study of Adenine Adsorption on Silver and Gold Surfaces. Journal of Physical Chemistry Letters, 2012, 3, 242-245.	4.6	95
6	The Infrared and Raman Spectra of Fullerene C70. DFT Calculations and Correlation with C60. Journal of Physical Chemistry A, 2002, 106, 1815-1823.	2.5	91
7	SERS and Computational Studies on MicroRNA Chains Adsorbed on Silver Surfaces. Journal of Physical Chemistry C, 2010, 114, 13730-13735.	3.1	67
8	Nitromethane Decomposition under High Static Pressure. Journal of Physical Chemistry B, 2010, 114, 9420-9428.	2.6	59
9	Immersive virtual reality in computational chemistry: Applications to the analysis of QM and MM data. International Journal of Quantum Chemistry, 2016, 116, 1731-1746.	2.0	52
10	Structure and Dynamics of Low-Density and High-Density Liquid Water at High Pressure. Journal of Physical Chemistry Letters, 2014, 5, 235-240.	4.6	50
11	A density functional study of the SERS spectra of pyridine adsorbed on silver clusters. Theoretical Chemistry Accounts, 2007, 117, 451-458.	1.4	49
12	Vibrational Frequencies of Fullerenes C₆₀ and C₇₀ under Pressure Studied with a Quantum Chemical Model Including Spatial Confinement Effects. Journal of Physical Chemistry A, 2014, 118, 5098-5111.	2.5	45
13	Anharmonic infrared and Raman spectra in Carâ€“Parrinello molecular dynamics simulations. Journal of Chemical Physics, 2008, 128, 224514.	3.0	44
14	Upgrading and Validation of the AMBER Force Field for Histidine and Cysteine Zinc(II)-Binding Residues in Sites with Four Protein Ligands. Journal of Chemical Information and Modeling, 2019, 59, 3803-3816.	5.4	42
15	Polarization response of water and methanol investigated by a polarizable force field and density functional theory calculations: Implications for charge transfer. Journal of Chemical Physics, 2005, 122, 074504.	3.0	40
16	A combined Raman, DFT and MD study of the solvation dynamics and the adsorption process of pyridine in silver hydrosols. Physical Chemistry Chemical Physics, 2006, 8, 171-178.	2.8	38
17	Electronic absorption spectra of pyridine and nicotine in aqueous solution with a combined molecular dynamics and polarizable QM/MM approach. Journal of Computational Chemistry, 2017, 38, 319-335.	3.3	38
18	Hydrogen Bond Dynamics of Methyl Acetate in Methanol. Journal of Physical Chemistry Letters, 2010, 1, 2951-2955.	4.6	36

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19	Raman and computational study of solvation and chemisorption of thiazole in silver hydrosol. Chemical Communications, 2011, 47, 3138.	4.1	36
20	Accurate prediction of bulk properties in hydrogen bonded liquids: amides as case studies. Physical Chemistry Chemical Physics, 2016, 18, 25342-25354.	2.8	36
21	Characterization of the non-covalent interaction between the PF-07321332 inhibitor and the SARS-CoV-2 main protease. Journal of Molecular Graphics and Modelling, 2022, 110, 108042.	2.4	34
22	Chemical Equilibrium Probed by Two-Dimensional IR Spectroscopy: Hydrogen Bond Dynamics of Methyl Acetate in Water. Journal of Physical Chemistry A, 2009, 113, 12783-12790.	2.5	31
23	Solvation Dynamics of Li+and Cl-Ions in Liquid Methanol. Journal of Physical Chemistry B, 2005, 109, 7475-7481.	2.6	30
24	Structural and Electronic Competing Mechanisms in the Formation of Amorphous Carbon Nitride by Compressing s-Triazine. Journal of Physical Chemistry C, 2015, 119, 28560-28569.	3.1	29
25	Virtual Double-System Single-Box: A Nonequilibrium Alchemical Technique for Absolute Binding Free Energy Calculations: Application to Ligands of the SARS-CoV-2 Main Protease. Journal of Chemical Theory and Computation, 2020, 16, 7160-7172.	5.3	27
26	Upgraded AMBER Force Field for Zinc-Binding Residues and Ligands for Predicting Structural Properties and Binding Affinities in Zinc-Proteins. ACS Omega, 2020, 5, 15301-15310.	3.5	27
27	Mycotoxins aptasensing: From molecular docking to electrochemical detection of deoxynivalenol. Bioelectrochemistry, 2021, 138, 107691.	4.6	27
28	Carâ€“Parrinello molecular dynamics on the SN2 reaction Clâ^'+CH3Br in water. Computational and Theoretical Chemistry, 2003, 630, 141-149.	1.5	24
29	Role of Surface Metal Clusters in SERS Spectra of Ligands Adsorbed on Ag Colloidal Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 762-767.	3.1	24
30	Structure and Dynamics of Br-Ion in Liquid Methanol. Journal of Physical Chemistry B, 2006, 110, 14923-14928.	2.6	23
31	DFT investigation on the SERS band at â^¼1025 cmâ^'1 of pyridine adsorbed on silver. Chemical Physics Letters, 2007, 436, 179-183.	2.6	23
32	Wavelet Transform for Spectroscopic Analysis: Application to Diols in Water. Journal of Chemical Theory and Computation, 2011, 7, 1109-1118.	5.3	23
33	Interaction of hydroxychloroquine with SARS-CoV2 functional proteins using all-atoms non-equilibrium alchemical simulations. Chemical Communications, 2020, 56, 8854-8856.	4.1	22
34	Ab- initio molecular dynamics study of the SN2 reaction Cl- + ClCH2CN. Physical Chemistry Chemical Physics, 2001, 3, 2559-2566.	2.8	21
35	Lithium Hydroxide Phase Transition under High Pressure: An Ab Initio Molecular Dynamics Study. ChemPhysChem, 2006, 7, 141-147.	2.1	20
36	Connecting the Water Phase Diagram to the Metastable Domain: High-Pressure Studies in the Supercooled Regime. Journal of Physical Chemistry Letters, 2014, 5, 3804-3809.	4.6	20

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37	Nitroimidazole-Based Ruthenium(II) Complexes: Playing with Structural Parameters to Design Photostable and Light-Responsive Antibacterial Agents. Inorganic Chemistry, 2022, 61, 6689-6694.	4.0	20
38	The solvation dynamics of Na+ and K+ ions in liquid methanol. Theoretical Chemistry Accounts, 2007, 118, 417-423.	1.4	19
39	Mechanism of the Ethylene Polymerization at Very High Pressure. Journal of Chemical Theory and Computation, 2008, 4, 646-651.	5.3	18
40	Spectroscopic properties with a combined approach of ab initio molecular dynamics and wavelet analysis. Journal of Molecular Structure, 2011, 993, 438-442.	3.6	18
41	Fine-tuning of atomic point charges: Classical simulations of pyridine in different environments. Chemical Physics Letters, 2017, 677, 120-126.	2.6	18
42	DFT calculations of the IR and Raman spectra of anthraquinone dyes and lakes. Journal of Raman Spectroscopy, 2018, 49, 668-683.	2.5	18
43	Ab Initio Molecular Dynamics Study of Mg²⁺ and Ca²⁺ Ions in Liquid Methanol. Journal of Chemical Theory and Computation, 2008, 4, 156-163.	5.3	17
44	High-Pressure Photoinduced Synthesis of Polynitrogen in Î´ and ïµ Nitrogen Crystals Substitutionally Doped with CO. Journal of Physical Chemistry C, 2015, 119, 130-140.	3.1	17
45	Solvation Dynamics and Adsorption on Ag Hydrosols of Oxazole: A Raman and Computational Study. Journal of Physical Chemistry A, 2009, 113, 15198-15205.	2.5	16
46	Pressure Dependence of Hydrogen-Bond Dynamics in Liquid Water Probed by Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 3579-3584.	4.6	16
47	Surfaceâ€enhanced Raman microâ€spectroscopy of DNA/RNA bases adsorbed on pyroxene rocks as a test ofin situsearch for life traces on Mars. Journal of Raman Spectroscopy, 2010, 41, 12-15.	2.5	15
48	Structural and Vibrational Properties of Arsenic Sulfides: Alacranite (As8S9). Journal of Physical Chemistry A, 2011, 115, 4558-4562.	2.5	15
49	Exploring the effect of Mg2+ substitution on amorphous calcium phosphate nanoparticles. Journal of Colloid and Interface Science, 2022, 606, 444-453.	9.4	15
50	Bifurcated Hydrogen Bond in Lithium Nitrate Trihydrate Probed by ab Initio Molecular Dynamics. Journal of Physical Chemistry A, 2012, 116, 2147-2153.	2.5	14
51	XP-PCM Calculations of High Pressure Structural and Vibrational Properties of P₄S₃. Journal of Physical Chemistry A, 2016, 120, 5136-5144.	2.5	14
52	Insights on the Realgar Crystal Under Pressure from XP-PCM and Periodic Model Calculations. Journal of Physical Chemistry A, 2017, 121, 8825-8834.	2.5	14
53	Binding Free Energies of Hostâ€“Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Theoretical Framework. Journal of Chemical Theory and Computation, 2017, 13, 5874-5886.	5.3	14
54	Binding Free Energies of Hostâ€“Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Illustrative Calculations and Numerical Validation. Journal of Chemical Theory and Computation, 2017, 13, 5887-5899.	5.3	14

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55	CarÃ¢â‚¬â€œParrinello molecular dynamics of the SN2 reaction ClÃ¢â‚¬â€œÃ¢â‚¬Â°+Ã¢â‚¬Â°Cl2CH2. Physical Chemistry Chemical Physics, 2001, 3, 4870-4873.	2.8	13
56	Positively Charged Active Sites for the Adsorption of Five-Membered Heterocycles on Silver Colloids. Journal of Physical Chemistry C, 2013, 117, 2328-2333.	3.1	13
57	Red lakes from Leonardo's Last Supper and other Old Master Paintings: Micro-Raman spectroscopy of anthraquinone pigments in paint cross-sections. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 222, 117273.	3.9	13
58	Structural and Spectroscopic Properties of Methanediol in Aqueous Solutions from Quantum Chemistry Calculations and Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2015, 119, 290-298.	2.5	11
59	New atomistic model of pyrrole with improved liquid state properties and structure. International Journal of Quantum Chemistry, 2018, 118, e25554.	2.0	11
60	Virtual Double-System Single-Box for Absolute Dissociation Free Energy Calculations in GROMACS. Journal of Chemical Information and Modeling, 2021, 61, 5320-5326.	5.4	11
61	Solid-State Phase Transition Induced by Pressure in LiOHÂ·H2O. Journal of Physical Chemistry B, 2006, 110, 13539-13546.	2.6	10
62	Hydrogen bond effects in the vibrational spectra of 1,3-propanediol in acetonitrile: Ab initio and experimental study. Journal of Chemical Physics, 2012, 137, 244501.	3.0	10
63	Evidence of a Lowâ€“High Density Turning Point in Liquid Water at Ordinary Temperature under Pressure: A Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2019, 10, 6414-6418.	4.6	9
64	Imidazole in Aqueous Solution: Hydrogen Bond Interactions and Structural Reorganization with Concentration. Journal of Physical Chemistry B, 2019, 123, 4055-4064.	2.6	9
65	Raman and infrared spectra of minerals from ab initio molecular dynamics simulations: The spodumene crystal. Journal of Molecular Structure, 2011, 993, 151-154.	3.6	8
66	SERS investigation of possible extraterrestrial life traces: Experimental adsorption of adenine on a Martian meteorite. Meteoritics and Planetary Science, 2012, 47, 853-860.	1.6	8
67	Vibronic coherences in light harvesting nanotubes: unravelling the role of dark states. Journal of Materials Chemistry C, 2022, 10, 7216-7226.	5.5	8
68	Competitive Solvation and Chemisorption in Silver Colloidal Suspensions. , 2012, , 39-44.		7
69	Thermal effects on the Clâ¯+ClCH2CN reaction by Car-Parrinello molecular dynamics. Journal of Chemical Physics, 2002, 117, 2199-2204.	3.0	6
70	Intramolecular solvation effects in the SN2 reaction Clâ¯+Cl(CH2)nCN. Journal of Chemical Physics, 2003, 119, 9063-9072.	3.0	6
71	Toward an Understanding of the Pressure Effect on the Intramolecular Vibrational Frequencies of Sulfur Hexafluoride. Journal of Physical Chemistry A, 2021, 125, 6362-6373.	2.5	6
72	Problems in molecular dynamics of condensed phases. Theoretical Chemistry Accounts, 2007, 117, 1105-1120.	1.4	5

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73	Computational Investigation of the Selective Cleavage of Diastereotopic Cyclopropane Bonds in 5-Spirocyclopropane Isoxazolidines Rearrangement. Journal of Organic Chemistry, 2019, 84, 6757-6764.	3.2	5
74	Computational Spectroscopy in Solution by Integration of Variational and Perturbative Approaches on Top of Clusterized Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 5747-5761.	5.3	5
75	Enhancing the Accuracy of Ab Initio Molecular Dynamics by Fine Tuning of Effective Two-Body Interactions: Acetonitrile as a Test Case. Journal of Physical Chemistry A, 2021, 125, 10475-10484.	2.5	4
76	Spectroscopy and monitoring of high pressure phenomena. Journal of Molecular Structure, 2009, 924-926, 2-8.	3.6	3
77	Nanostructured Ag Platforms as Biosensors of Nucleobase Chains. Journal of Nanoscience and Nanotechnology, 2011, 11, 8763-8767.	0.9	3
78	Fabrication of nanostructured silver substrates for surface-enhanced Raman spectroscopy. Journal of Nanoparticle Research, 2011, 13, 5863-5871.	1.9	3
79	Identification of Di(oxymethylene)glycol in the Raman Spectrum of Formaldehyde Aqueous Solutions by ab Initio Molecular Dynamics Simulations and Quantum Chemistry Calculations. Journal of Physical Chemistry A, 2015, 119, 9785-9793.	2.5	3
80	â€œCyclopropylidene Effectâ€•in the 1,3-Dipolar Cycloaddition of Nitrones to Alkylidene Cyclopropanes: A Computational Rationalization. Journal of Physical Chemistry A, 2021, 125, 3892-3899.	2.5	3
81	A multi-technique approach to predicting the molecular structure of cuprizone in the gas phase and in the crystalline state. CrystEngComm, 2008, , .	2.6	2
82	Photochemical Reactivity of 1,6-Methano[10]annulene. Journal of Physical Chemistry A, 2017, 121, 4412-4421.	2.5	2
83	Spectroscopic studies on antimalarial Artesunate: Raman and surface-enhanced Raman scattering and adsorption geometries of Artesunate on silver nanoparticles. Journal of Molecular Structure, 2021, 1224, 129020.	3.6	2
84	Adsorption Geometry of Alizarin on Silver Nanoparticles: A Computational and Spectroscopic Study. Nanomaterials, 2021, 11, 860.	4.1	2
85	Ethanol electro-oxidation reaction on the Pd(111) surface in alkaline media: insights from quantum and molecular mechanics. Physical Chemistry Chemical Physics, 2022, , .	2.8	2
86	Modification of local and collective dynamics of water in perchlorate solution, induced by pressure and concentration. Journal of Molecular Liquids, 2021, 337, 116273.	4.9	1
87	Development, Validation, and Pilot Application of a Generalized Fluctuating Charge Model for Computational Spectroscopy in Solution. ACS Omega, 2022, 7, 13382-13394.	3.5	1
88	Conformational and solvent effects in structural and spectroscopic properties of 2-hydroxyethyl methacrylate and acrylic acid. Journal of Molecular Liquids, 2022, 360, 119428.	4.9	1
89	Surface-Enhanced Raman Scattering Investigation of Nucleobases Adsorbed on Samples of Martian Analogue Material. Spectroscopy Letters, 2011, 44, 580-584.	1.0	0
90	Correspondence between light-absorption spectrum and nonequilibrium work distribution as a mean to access free energy differences between electronic states. Journal of Chemical Physics, 2018, 149, 084101.	3.0	0

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91	Regioselective Deuteration of a 3,4â€Dialkoxypyrroline Nâ€Oxide and Synthesis of 8aâ€dâ€Indolizidines. European Journal of Organic Chemistry, 2020, 2020, 3423-3429.	2.4	0