Chiara Cappelli

List of Publications by Year
in descending order

119 papers	4,323 citations	100601 38 h-index	150775 59 g-index
124 all docs	124 docs citations	124 times ranked	3698 citing authors

#	Article	IF	Citations
1	Ring Vibrations to Sense Anionic Ibuprofen in Aqueous Solution as Revealed by Resonance Raman. Molecules, 2022, 27, 442.	1.7	13
2	Absorption Properties of Large Complex Molecular Systems: The DFTB/Fluctuating Charge Approach. Journal of Chemical Theory and Computation, 2022, 18, 1765-1779.	2.3	8
3	In silico design of graphene plasmonic hot-spots. Nanoscale Advances, 2022, 4, 2294-2302.	2.2	6
4	Amide Spectral Fingerprints are Hydrogen Bonding-Mediated. Journal of Physical Chemistry Letters, 2022, 13, 6200-6207.	2.1	9
5	Multilevel Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 791-803.	2.3	21
6	A polarizable three-layer frozen density embedding/molecular mechanics approach. Journal of Chemical Physics, 2021, 154, 164107.	1.2	7
7	Exploring Biases in Atom Probe Tomography Compositional Analysis of Minerals. Geostandards and Geoanalytical Research, 2021, 45, 457-476.	1.7	7
8	Thermodynamics and Intermolecular Interactions during the Insertion of Anionic Naproxen into Model Cell Membranes. Journal of Physical Chemistry B, 2021, 125, 10383-10391.	1.2	13
9	A molecular twist on hydrophobicity. Chemical Science, 2021, 12, 9233-9245.	3.7	22
10	Quantum Mechanics/Fluctuating Charge Protocol to Compute Solvatochromic Shifts. Journal of Chemical Theory and Computation, 2021, 17, 7146-7156.	2.3	15
11	Atom Probe Tomography Analysis of Mica. Microscopy and Microanalysis, 2021, , 1-14.	0.2	2
12	Going Beyond the Limits of Classical Atomistic Modeling of Plasmonic Nanostructures. Journal of Physical Chemistry C, 2021, 125, 23848-23863.	1.5	11
13	Evolution of Bonding during the Insertion of Anionic Ibuprofen into Model Cell Membranes. Journal of Physical Chemistry B, 2020, 124, 79-90.	1.2	21
14	Calculation of Linear and Non-linear Electric Response Properties of Systems in Aqueous Solution: A Polarizable Quantum/Classical Approach with Quantum Repulsion Effects. Journal of Chemical Theory and Computation, 2020, 16, 6993-7004.	2.3	16
15	Theory and algorithms for chiroptical properties and spectroscopies of aqueous systems. Physical Chemistry Chemical Physics, 2020, 22, 22864-22879.	1.3	29
16	Biotite reactivity in nitric and oxalic acid at low temperature and acid pH from surface and bulk dissolution measurements. Chemical Geology, 2020, 554, 119806.	1.4	4
17	Molecular spectroscopy of aqueous solutions: a theoretical perspective. Chemical Society Reviews, 2020, 49, 5664-5677.	18.7	55
18	Graphene Plasmonics: Fully Atomistic Approach for Realistic Structures. Journal of Physical Chemistry Letters, 2020, 11, 7595-7602.	2.1	13

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19	Simulating Absorption Spectra of Flavonoids in Aqueous Solution: A Polarizable QM/MM Study. Molecules, 2020, 25, 5853.	1.7	15
20	Effect of crystallographic orientation on atom probe tomography geochemical data?. Micron, 2020, 137, 102910.	1.1	8
21	In Situ Geochemical Analysis of Organics in Growth Lines of Antarctic Scallop Shells: Implications for Sclerochronology. Minerals (Basel, Switzerland), 2020, 10, 529.	0.8	8
22	Absorption spectra of xanthines in aqueous solution: a computational study. Physical Chemistry Chemical Physics, 2020, 22, 5929-5941.	1.3	23
23	Simulating vertical excitation energies of solvated dyes: From continuum to polarizable discrete modeling. International Journal of Quantum Chemistry, 2019, 119, e25684.	1.0	37
24	Atom Probe Tomography (APT) Characterization of Organics Occluded in Single Calcite Crystals: Implications for Biomineralization Studies. Journal of Carbon Research, 2019, 5, 50.	1.4	8
25	The Role of pH, Temperature, and NH₄⁺ during Mica Weathering. ACS Earth and Space Chemistry, 2019, 3, 2613-2622.	1.2	9
26	Calculation of IR Spectra with a Fully Polarizable QM/MM Approach Based on Fluctuating Charges and Fluctuating Dipoles. Journal of Chemical Theory and Computation, 2019, 15, 5495-5507.	2.3	35
27	Quantum Confinement Effects on Solvatochromic Shifts of Molecular Solutes. Journal of Physical Chemistry Letters, 2019, 10, 5823-5829.	2.1	31
28	A combined experimental and theoretical study of optical rotatory dispersion for (R)-glycidyl methyl ether in aqueous solution. Physical Chemistry Chemical Physics, 2019, 21, 3644-3655.	1.3	30
29	Interplay between conformational and solvent effects in UV-visible absorption spectra: curcumin tautomers as a case study. Physical Chemistry Chemical Physics, 2019, 21, 15504-15514.	1.3	47
30	Fully Polarizable QM/Fluctuating Charge Approach to Two-Photon Absorption of Aqueous Solutions. Journal of Chemical Theory and Computation, 2019, 15, 4056-4068.	2.3	24
31	Polarizable QM/MM Approach with Fluctuating Charges and Fluctuating Dipoles: The QM/FQFÎ¼ Model. Journal of Chemical Theory and Computation, 2019, 15, 2233-2245.	2.3	55
32	Effective yet reliable computation of hyperfine coupling constants in solution by a QM/MM approach: Interplay between electrostatics and non-electrostatic effects. Journal of Chemical Physics, 2019, 150, 124102.	1.2	42
33	A classical picture of subnanometer junctions: an atomistic Drude approach to nanoplasmonics. Nanoscale, 2019, 11, 6004-6015.	2.8	25
34	Electronic transitions for a fully polarizable QM/MM approach based on fluctuating charges and fluctuating dipoles: Linear and corrected linear response regimes. Journal of Chemical Physics, 2019, 151, 174104.	1.2	42
35	Effective computational route towards vibrational optical activity spectra of chiral molecules in aqueous solution. Physical Chemistry Chemical Physics, 2018, 20, 9181-9197.	1.3	46
36	Montmorillonite dissolution kinetics: Experimental and reactive transport modeling interpretation. Geochimica Et Cosmochimica Acta, 2018, 227, 96-122.	1.6	14

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37	Evaluation of Hyperpolarizability from the Solvatochromic Method: Thiophene Containing Pushâ€“Pull Cationic Dyes as a Case Study. Journal of Physical Chemistry C, 2018, 122, 2285-2296.	1.5	32
38	A 4,4â€²-bis(2-benzoxazolyl)stilbene luminescent probe: assessment of aggregate formation through photophysics experiments and quantum-chemical calculations. Physical Chemistry Chemical Physics, 2018, 20, 26249-26258.	1.3	4
39	On the nature of charge-transfer excitations for molecules in aqueous solution: a polarizable QM/MM study. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	14
40	A polarizable embedding approach to second harmonic generation (SHG) of molecular systems in aqueous solutions. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	28
41	A General Route to Include Pauli Repulsion and Quantum Dispersion Effects in QM/MM Approaches. Journal of Chemical Theory and Computation, 2017, 13, 4854-4870.	2.3	62
42	Polarizable Embedding Approach for the Analytical Calculation of Raman and Raman Optical Activity Spectra of Solvated Systems. Journal of Chemical Theory and Computation, 2017, 13, 4421-4435.	2.3	39
43	Understanding the interplay between the solvent and nuclear rearrangements in the negative solvatochromism of a pushâ€“pull flexible quinolinium cation. Physical Chemistry Chemical Physics, 2017, 19, 32544-32555.	1.3	7
44	Integrated QM/polarizable MM/continuum approaches to model chiroptical properties of strongly interacting soluteâ€“solvent systems. International Journal of Quantum Chemistry, 2016, 116, 1532-1542.	1.0	75
45	In situ observation of biotite (001) surface dissolution at pH 1 and 9.5 by advanced optical microscopy. Beilstein Journal of Nanotechnology, 2015, 6, 665-673.	1.5	4
46	Origin invariance in vibrational resonance Raman optical activity. Journal of Chemical Physics, 2015, 142, 174101.	1.2	25
47	The Electronic Circular Dichroism of Nicotine in Aqueous Solution: A Test Case for Continuum and Mixed Explicit-Continuum Solvation Approaches. Journal of Physical Chemistry A, 2015, 119, 5396-5404.	1.1	33
48	Optical rotatory dispersion of methyloxirane in aqueous solution: assessing the performance of density functional theory in combination with a fully polarizable QM/MM/PCM approach. Optical Materials Express, 2015, 5, 196.	1.6	23
49	A benchmark study of electronic excitation energies, transition moments, and excited-state energy gradients on the nicotine molecule. Journal of Chemical Physics, 2014, 141, 224114.	1.2	23
50	Stereoelectronic, Vibrational, and Environmental Contributions to Polarizabilities of Large Molecular Systems: A Feasible Anharmonic Protocol. Journal of Chemical Theory and Computation, 2014, 10, 2456-2464.	2.3	35
51	A Robust and Effective Time-Independent Route to the Calculation of Resonance Raman Spectra of Large Molecules in Condensed Phases with the Inclusion of Duschinsky, Herzbergâ€“Teller, Anharmonic, and Environmental Effects. Journal of Chemical Theory and Computation, 2014, 10, 346-363.	2.3	71
52	Cobalt complexes able to bind dioxygen: Thermodynamic studies and DFT calculations. Inorganica Chimica Acta, 2014, 417, 230-238.	1.2	6
53	An integrated computational tool to model the broadening of the absorption bands of flexible dyes in solution: cationic chromophores as test cases. Physical Chemistry Chemical Physics, 2014, 16, 26963-26973.	1.3	17
54	Ultrafast resonance energy transfer in the umbelliferoneâ€“alizarin bichromophore. Physical Chemistry Chemical Physics, 2014, 16, 10059-10074.	1.3	12

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55	Combination of Transient 2D-IR Experiments and Ab Initio Computations Sheds Light on the Formation of the Charge-Transfer State in Photoexcited Carbonyl Carotenoids. Journal of Physical Chemistry B, 2014, 118, 9613-9630.	1.2	17
56	Development of a Virtual Spectrometer for Chiroptical Spectroscopies: The Case of Nicotine. Chirality, 2013, 25, 701-708.	1.3	22
57	Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds. Journal of Chemical Physics, 2013, 139, 074310.	1.2	72
58	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.	1.2	9
59	Computational Design, Synthesis, and Mechanochromic Properties of New Thiopheneâ€Based Ï€â€Conjugated Chromophores. Chemistry - A European Journal, 2013, 19, 1996-2004.	1.7	43
60	The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?. Journal of Chemical Theory and Computation, 2013, 9, 1880-1884.	2.3	76
61	In Situ Observation of Biotite Dissolution at pH 1 Using Advanced Optical Microscopy. Crystal Growth and Design, 2013, 13, 2880-2886.	1.4	12
62	Duschinsky, Herzbergâ€“Teller, and Multiple Electronic Resonance Interferential Effects in Resonance Raman Spectra and Excitation Profiles. The Case of Pyrene. Journal of Chemical Theory and Computation, 2013, 9, 3597-3611.	2.3	60
63	Tuning of NMR and EPR parameters by vibrational averaging and environmental effects: an integrated computational approach. Molecular Physics, 2013, 111, 1345-1354.	0.8	12
64	Vertical Electronic Excitations in Solution with the EOM-CCSD Method Combined with a Polarizable Explicit/Implicit Solvent Model. Journal of Chemical Theory and Computation, 2013, 9, 3035-3042.	2.3	48
65	Effective time-independent studies on resonance Raman spectroscopy of trans-stilbene including the Duschinsky effect. Molecular Physics, 2013, 111, 1511-1525.	0.8	4
66	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. Journal of Chemical Physics, 2013, 139, 164302.	1.2	36
67	A gauge invariant multiscale approach to magnetic spectroscopies in condensed phase: General three-layer model, computational implementation and pilot applications. Journal of Chemical Physics, 2013, 138, 234108.	1.2	47
68	Toward Ab Initio Anharmonic Vibrational Circular Dichroism Spectra in the Condensed Phase. Journal of Physical Chemistry Letters, 2012, 3, 1766-1773.	2.1	50
69	Toward an Accurate Modeling of Optical Rotation for Solvated Systems: Anharmonic Vibrational Contributions Coupled to the Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2012, 8, 585-597.	2.3	46
70	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. Physical Chemistry Chemical Physics, 2012, 14, 12404.	1.3	128
71	Linear Response Theory and Electronic Transition Energies for a Fully Polarizable QM/Classical Hamiltonian. Journal of Chemical Theory and Computation, 2012, 8, 4153-4165.	2.3	111
72	Analytical First and Second Derivatives for a Fully Polarizable QM/Classical Hamiltonian. Journal of Chemical Theory and Computation, 2012, 8, 4270-4278.	2.3	68

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73	Modelling vibrational coupling in DNA oligomers: a computational strategy combining QM and continuum solvation models. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	13
74	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.	0.5	64
75	Effect of lactate, glycine, and citrate on the kinetics of montmorillonite dissolution. American Mineralogist, 2011, 96, 768-780.	0.9	24
76	Effective Time-Independent Calculations of Vibrational Resonance Raman Spectra of Isolated and Solvated Molecules Including Duschinsky and Herzbergâ€“Teller Effects. Journal of Chemical Theory and Computation, 2011, 7, 1824-1839.	2.3	77
77	Cavity field effects within a polarizable continuum model of solvation: Application to the calculation of electronic circular dichroism spectra of Râ€(+)â€3â€methylâ€cyclopentanone. International Journal of Quantum Chemistry, 2011, 111, 826-838.	1.0	20
78	David Bishop's approach to vibrational dynamic contributions to molecular properties: Application to Jones and magnetoelectric birefringences in diatomic molecules. International Journal of Quantum Chemistry, 2011, 111, 760-771.	1.0	2
79	Modeling solvent effects on chiroptical properties. Chirality, 2011, 23, 717-729.	1.3	106
80	Towards an accurate description of anharmonic infrared spectra in solution within the polarizable continuum model: Reaction field, cavity field and nonequilibrium effects. Journal of Chemical Physics, 2011, 135, 104505.	1.2	48
81	On the Calculation of Vibrational Frequencies for Molecules in Solution Beyond the Harmonic Approximation. Journal of Chemical Theory and Computation, 2010, 6, 1660-1669.	2.3	52
82	Toward a Quantum-Mechanical Description of 2D-IR Spectra of Solvated Systems: The Vibrational Mode Coupling within A Polarizable Continuum Model. Journal of Physical Chemistry B, 2010, 114, 4924-4930.	1.2	7
83	Structures and Properties of Electronically Excited Chromophores in Solution from the Polarizable Continuum Model Coupled to the Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 3009-3020.	1.1	173
84	Ab Initio Study of the Magnetoâ€Optical Rotation of Diastereoisomers. ChemPhysChem, 2008, 9, 462-469.	1.0	1
85	Modulation of the Optical Response of Polyethylene Films Containing Luminescent Perylene Chromophores. Journal of Physical Chemistry B, 2008, 112, 3668-3679.	1.2	115
86	How the Environment Controls Absorption and Fluorescence Spectra of PRODAN:â€‰ A Quantum-Mechanical Study in Homogeneous and Heterogeneous Media. Journal of Physical Chemistry B, 2008, 112, 414-423.	1.2	65
87	Modeling the Solvation of Peptides. The Case of (s)-N-Acetylproline Amide in Liquid Water. Journal of Physical Chemistry B, 2008, 112, 3441-3450.	1.2	26
88	Modification and photostabilization of low density polyethylene film by photodecomposition of various diazo-compounds and methyl azidocarboxylate. Polymer Degradation and Stability, 2007, 92, 849-858.	2.7	10
89	Conferring dichroic properties and optical responsiveness to polyolefins through organic chromophores and metal nanoparticles. Progress in Organic Coatings, 2007, 58, 105-116.	1.9	29
90	A quantum mechanical polarizable continuum model for the calculation of resonance Raman spectra in condensed phase. Theoretical Chemistry Accounts, 2007, 117, 1029-1039.	0.5	46

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91	Characterization of Supramolecular Polyphenolâ^'Chromium(III) Clusters by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 13227-13234.	1.2	10
92	Solvent Effects on Raman Optical Activity Spectra Calculated Using the Polarizable Continuum Model. Journal of Physical Chemistry A, 2006, 110, 2807-2815.	1.1	59
93	Dichroic Properties of Bis(benzoxazolyl)stilbene and Bis(benzoxazolyl)thiophene Dispersed into Oriented Polyethylene Films:â€‰ A Combined Experimental and Density Functional Theory Approach. Journal of Physical Chemistry B, 2006, 110, 3127-3134.	1.2	37
94	Towards the design of highly selective recognition sites into molecular imprinting polymers: A computational approach. Biosensors and Bioelectronics, 2006, 22, 153-163.	5.3	49
95	Density-functional-theory study of the electric-field-induced second harmonic generation (EFISHG) of pushâ€“pull phenylpolyenes in solution. Chemical Physics Letters, 2006, 425, 267-272.	1.2	99
96	Computational study of conformational and chiroptical properties of (2R,3S,4R)-(+)-3,3â€²,4,4â€²,7-flavanpentol. Chirality, 2005, 17, 577-589.	1.3	20
97	Infrared linear dichroism in stretched films: Quantum mechanical approach within the polarizable continuum model. International Journal of Quantum Chemistry, 2005, 104, 716-726.	1.0	9
98	Effect of the environment on vibrational infrared and circular dichroism spectra of (s)-proline. International Journal of Quantum Chemistry, 2005, 104, 744-757.	1.0	26
99	A computational study of some electric and magnetic properties of gaseous BF3 and BCl3. Journal of Chemical Physics, 2005, 123, 114307.	1.2	9
100	Density-functional theory study of electric and magnetic properties of hexafluorobenzene in the vapor phase. Journal of Chemical Physics, 2005, 122, 234314.	1.2	27
101	Toward the Supramolecular Structure of Collagen:Â A Molecular Dynamics Approach. Journal of Physical Chemistry B, 2005, 109, 11389-11398.	1.2	28
102	Understanding the Accelerating Effect of Îµ-Caprolactam on the Formation of Urethane Linkages. Macromolecules, 2005, 38, 1385-1394.	2.2	12
103	Quantum Mechanical Polarizable Continuum Model Approach to the Kerr Effect of Pure Liquids. Journal of Physical Chemistry B, 2005, 109, 18706-18714.	1.2	29
104	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.	1.1	71
105	Density-functional and electron correlated study of five linear birefringencesâ€”Kerr, Cottonâ€“Mouton, Buckingham, Jones, and magnetoelectricâ€”in gaseous benzene. Journal of Chemical Physics, 2004, 121, 8814-8830.	1.2	30
106	Second-order MÃ¸llerâ€“Plesset second derivatives for the polarizable continuum model: theoretical bases and application to solvent effects in electrophilic bromination of ethylene. Theoretical Chemistry Accounts, 2004, 111, 66-77.	0.5	13
107	Understanding the Structural and Binding Properties of Collagen:â€‰ A Theoretical Perspective. Journal of Physical Chemistry B, 2004, 108, 10101-10112.	1.2	39
108	Prediction of Solvent Effects on Vibrational Absorption Intensities and Raman Activities in Solution within the Polarizable Continuum Model:â€‰ A Study on Pushâ^'Pull Molecules. Journal of Physical Chemistry A, 2003, 107, 10261-10271.	1.1	13

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109	Combining Theory and Experiment to Study the Photooxidation of Polyethylene and Polypropylene. Journal of Physical Chemistry B, 2003, 107, 11880-11888.	1.2	40
110	The Cottonâ€“Mouton effect of furan and its homologues in the gas phase, for the pure liquids and in solution. Journal of Chemical Physics, 2003, 118, 10712-10724.	1.2	37
111	Vibrational Circular Dichroism within the Polarizable Continuum Model:Â A Theoretical Evidence of Conformation Effects and Hydrogen Bonding for (S)-(âˆ')-3-Butyn-2-ol in CCl4Solution. Journal of Physical Chemistry A, 2002, 106, 12331-12339.	1.1	83
112	Molecular properties in solution described with a continuum solvation model. Physical Chemistry Chemical Physics, 2002, 4, 5697-5712.	1.3	277
113	Theoretical Approach to the Calculation of Vibrational Raman Spectra in Solution within the Polarizable Continuum Model. Journal of Physical Chemistry A, 2001, 105, 8310-8316.	1.1	53
114	Solvent Effects on trans/gauche Conformational Equilibria of Substituted Chloroethanes:â€‰ a Polarizable Continuum Model Study. Journal of Physical Chemistry A, 2001, 105, 10807-10815.	1.1	42
115	The Cottonâ€“Mouton effect of gaseous N2, CO, CO2, N2O, OCS and CS2: a density functional approach to high-order mixed electric and magnetic properties. Chemical Physics Letters, 2001, 346, 251-258.	1.2	16
116	Solvent effects on vibrational modes: ab-initio calculations, scaling and solvent functions with applications to the carbonyl stretch of dialkyl ketones. Computational and Theoretical Chemistry, 2001, 544, 191-203.	1.5	23
117	Electronic and vibrational dynamic solvent effects on Raman spectra. Journal of Chemical Physics, 2001, 115, 5531-5535.	1.2	38
118	Nonequilibrium formulation of infrared frequencies and intensities in solution: Analytical evaluation within the polarizable continuum model. Journal of Chemical Physics, 2000, 113, 11270-11279.	1.2	69
119	Properties and Spectroscopies. , 0, , 125-312.		3