

Roberto Cammi

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150
papers

24,802
citations

50
h-index

156
g-index

156
ext. papers

26,971
ext. citations

3.9
avg, IF

7.06
L-index

#	Paper	IF	Citations
150	Quantum mechanical continuum solvation models. <i>Chemical Reviews</i> , 2005 , 105, 2999-3093	68.1	11786
149	Ab initio study of solvated molecules: a new implementation of the polarizable continuum model. <i>Chemical Physics Letters</i> , 1996 , 255, 327-335	2.5	2731
148	Remarks on the use of the apparent surface charges (ASC) methods in solvation problems: Iterative versus matrix-inversion procedures and the renormalization of the apparent charges. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1449-1458	3.5	1044
147	Geometries and properties of excited states in the gas phase and in solution: theory and application of a time-dependent density functional theory polarizable continuum model. <i>Journal of Chemical Physics</i> , 2006 , 124, 94107	3.9	989
146	Polarizable Continuum Model (PCM) Calculations of Solvent Effects on Optical Rotations of Chiral Molecules. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 6102-6113	2.8	494
145	Fast Evaluation of Geometries and Properties of Excited Molecules in Solution: A Tamm-Dancoff Model with Application to 4-Dimethylaminobenzonitrile. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 5637-5637	2.8	484
144	Formation and relaxation of excited states in solution: a new time dependent polarizable continuum model based on time dependent density functional theory. <i>Journal of Chemical Physics</i> , 2006 , 124, 124520	3.9	407
143	Recent Advances in the Description of Solvent Effects with the Polarizable Continuum Model. <i>Advances in Quantum Chemistry</i> , 1998 , 32, 227-261	1.4	373
142	Excited states and solvatochromic shifts within a nonequilibrium solvation approach: A new formulation of the integral equation formalism method at the self-consistent field, configuration interaction, and multiconfiguration self-consistent field level. <i>Journal of Chemical Physics</i> , 1998 , 109, 2798-2807	3.9	326
141	Linear response theory for the polarizable continuum model. <i>Journal of Chemical Physics</i> , 1999 , 110, 9873-9886	3.9	262
140	Molecular properties in solution described with a continuum solvation model. <i>Physical Chemistry Chemical Physics</i> , 2002 , 4, 5697-5712	3.6	261
139	Electronic excitation energies of molecules in solution: state specific and linear response methods for nonequilibrium continuum solvation models. <i>Journal of Chemical Physics</i> , 2005 , 122, 104513	3.9	240
138	Second-Order Møller-Plesset Analytical Derivatives for the Polarizable Continuum Model Using the Relaxed Density Approach. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 9100-9108	2.8	215
137	Electronic excitation energies of molecules in solution within continuum solvation models: investigating the discrepancy between state-specific and linear-response methods. <i>Journal of Chemical Physics</i> , 2005 , 123, 134512	3.9	172
136	Theoretical chemistry in solution. Some results and perspectives of the continuum methods and in particular of the polarizable continuum model. <i>Computational and Theoretical Chemistry</i> , 1991 , 234, 401-424		169
135	Structures and properties of electronically excited chromophores in solution from the polarizable continuum model coupled to the time-dependent density functional theory. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 3009-20	2.8	158
134	Calculation of pKa values of nucleobases and the guanine oxidation products guanidinohydantoin and spiroiminodihydantoin using density functional theory and a polarizable continuum model. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 16860-73	3.4	157

133	Excitation energy transfer (EET) between molecules in condensed matter: a novel application of the polarizable continuum model (PCM). <i>Journal of Chemical Physics</i> , 2004 , 120, 7029-40	3.9	155
132	How solvent controls electronic energy transfer and light harvesting. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 6978-82	3.4	150
131	Analytical Hartree-Fock calculation of the dynamical polarizabilities α and β of molecules in solution. <i>Journal of Chemical Physics</i> , 1996 , 105, 10556-10564	3.9	142
130	Analytical derivatives for molecular solutes. III. Hartree-Fock static polarizability and hyperpolarizabilities in the polarizable continuum model. <i>Journal of Chemical Physics</i> , 1996 , 104, 4611-4620	3.9	140
129	Analytical derivatives for molecular solutes. I. Hartree-Fock energy first derivatives with respect to external parameters in the polarizable continuum model. <i>Journal of Chemical Physics</i> , 1994 , 100, 7495-7502	3.9	117
128	An Attempt To Bridge the Gap between Computation and Experiment for Nonlinear Optical Properties: "Macroscopic Susceptibilities in Solution" <i>Journal of Physical Chemistry A</i> , 2000 , 104, 4690-4698	3.8	114
127	On the Calculation of Local Field Factors for Microscopic Static Hyperpolarizabilities of Molecules in Solution with the Aid of Quantum-Mechanical Methods. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 870-875	3.8	107
126	Analytical free energy second derivatives with respect to nuclear coordinates: Complete formulation for electrostatic continuum solvation models. <i>Journal of Chemical Physics</i> , 1999 , 110, 6858-6870	3.9	107
125	Multiconfigurational self-consistent field linear response for the polarizable continuum model: Theory and application to ground and excited-state polarizabilities of para-nitroaniline in solution. <i>Journal of Chemical Physics</i> , 2003 , 119, 5818-5827	3.9	104
124	How solvent controls electronic energy transfer and light harvesting: toward a quantum-mechanical description of reaction field and screening effects. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 13253-65	3.4	102
123	Medium effects on the properties of chemical systems: An overview of recent formulations in the polarizable continuum model (PCM). <i>International Journal of Quantum Chemistry</i> , 1999 , 75, 783-803	2.1	99
122	Analytical first derivatives of molecular surfaces with respect to nuclear coordinates. <i>Journal of Computational Chemistry</i> , 1996 , 17, 57-73	3.5	98
121	Nuclear magnetic shieldings in solution: Gauge invariant atomic orbital calculation using the polarizable continuum model. <i>Journal of Chemical Physics</i> , 1999 , 110, 7627-7638	3.9	97
120	Nonequilibrium solvation theory for the polarizable continuum model: A new formulation at the SCF level with application to the case of the frequency-dependent linear electric response function. <i>International Journal of Quantum Chemistry</i> , 1995 , 56, 465-474	2.1	94
119	Counterpoise corrections to the interaction energy components in bimolecular complexes. <i>Theoretica Chimica Acta</i> , 1985 , 68, 271-283		91
118	Modeling solvent effects on chiroptical properties. <i>Chirality</i> , 2011 , 23, 717-29	2.1	90
117	Solvent Effects on Linear and Nonlinear Optical Properties of Donor-Acceptor Polyenes: Investigation of Electronic and Vibrational Components in Terms of Structure and Charge Distribution Changes. <i>Journal of the American Chemical Society</i> , 1998 , 120, 8834-8847	16.4	90
116	Analytical derivatives for molecular solutes. II. Hartree-Fock energy first and second derivatives with respect to nuclear coordinates. <i>Journal of Chemical Physics</i> , 1994 , 101, 3888-3897	3.9	88

115	Vibrational Circular Dichroism within the Polarizable Continuum Model: A Theoretical Evidence of Conformation Effects and Hydrogen Bonding for (S)-1,3-Butyn-2-ol in CCl ₄ Solution. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 12331-12339	2.8	79
114	On the Calculation of Infrared Intensities in Solution within the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 9874-9879	2.8	77
113	Squeezing All Elements in the Periodic Table: Electron Configuration and Electronegativity of the Atoms under Compression. <i>Journal of the American Chemical Society</i> , 2019 , 141, 10253-10271	16.4	76
112	The Hartree-Fock calculation of the magnetic properties of molecular solutes. <i>Journal of Chemical Physics</i> , 1998 , 109, 3185-3196	3.9	73
111	Symmetry-adapted cluster and symmetry-adapted cluster-configuration interaction method in the polarizable continuum model: theory of the solvent effect on the electronic excitation of molecules in solution. <i>Journal of Chemical Physics</i> , 2010 , 133, 024104	3.9	70
110	Quantum cluster theory for the polarizable continuum model. I. The CCSD level with analytical first and second derivatives. <i>Journal of Chemical Physics</i> , 2009 , 131, 164104	3.9	69
109	A second-order, quadratically convergent multiconfigurational self-consistent field polarizable continuum model for equilibrium and nonequilibrium solvation. <i>Journal of Chemical Physics</i> , 2002 , 117, 13-26	3.9	65
108	How the environment controls absorption and fluorescence spectra of PRODAN: a quantum-mechanical study in homogeneous and heterogeneous media. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 414-23	3.4	63
107	Solvent Effects on the Indirect Spin-Spin Coupling Constants of Benzene: The DFT-PCM Approach. <i>International Journal of Molecular Sciences</i> , 2003 , 4, 119-134	6.3	63
106	Nonequilibrium formulation of infrared frequencies and intensities in solution: Analytical evaluation within the polarizable continuum model. <i>Journal of Chemical Physics</i> , 2000 , 113, 11270-11279	3.9	63
105	A polarizable continuum model for molecules at diffuse interfaces. <i>Journal of Chemical Physics</i> , 2004 , 120, 3893-907	3.9	62
104	The Effect of Pressure on Organic Reactions in Fluids-a New Theoretical Perspective. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 11126-11142	16.4	55
103	Calculation and analysis of the harmonic vibrational frequencies in molecules at extreme pressure: methodology and diborane as a test case. <i>Journal of Chemical Physics</i> , 2012 , 137, 154112	3.9	54
102	Ultrafast light harvesting dynamics in the cryptophyte phycocyanin 645. <i>Photochemical and Photobiological Sciences</i> , 2007 , 6, 964-75	4.2	51
101	Nonequilibrium solvation for vertical photoemission and photoabsorption processes using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model. <i>Journal of Chemical Physics</i> , 2011 , 134, 104109	3.9	50
100	Towards the elaboration of a QM method to describe molecular solutes under the effect of a very high pressure. <i>Chemical Physics</i> , 2008 , 344, 135-141	2.3	50
99	Theoretical Approach to the Calculation of Vibrational Raman Spectra in Solution within the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 8310-8316	2.8	49
98	Mechanistic Insights into Acetophenone Transfer Hydrogenation Catalyzed by Half-Sandwich Ruthenium(II) Complexes Containing 2-(Diphenylphosphanyl)aniline [A Combined Experimental and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2008 , 2008, 4462-4473	2.3	44

97	The effect of full and limited counterpoise corrections with different basis sets on the energy and the equilibrium distance of hydrogen bonded dimers. <i>International Journal of Quantum Chemistry</i> , 1987 , 32, 207-226	2.1	44
96	A quantum mechanical polarizable continuum model for the calculation of resonance Raman spectra in condensed phase. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 1029-1039	1.9	41
95	On the evaluation of the solvent polarization apparent charges in the polarizable continuum model: A new formulation. <i>Journal of Computational Chemistry</i> , 1995 , 16, 20-30	3.5	40
94	Coupled-cluster theories for the polarizable continuum model. II. Analytical gradients for excited states of molecular solutes by the equation of motion coupled-cluster method. <i>International Journal of Quantum Chemistry</i> , 2010 , 110, 3040-3052	2.1	39
93	The Cotton-Mouton effect of furan and its homologues in the gas phase, for the pure liquids and in solution. <i>Journal of Chemical Physics</i> , 2003 , 118, 10712-10724	3.9	36
92	Vibrational frequencies of fullerenes C60 and C70 under pressure studied with a quantum chemical model including spatial confinement effects. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 5098-111	2.8	35
91	Modern Theories of Continuum Models1-123		35
90	Quantum-Mechanical Continuum Solvation Study of the Polarizability of Halides at the Water/Air Interface. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 13796-13806	3.4	34
89	Counterpoise corrections to the evaluation of the bimolecular interaction energy components. <i>Theoretica Chimica Acta</i> , 1986 , 69, 11-22		33
88	A new extension of the polarizable continuum model: Toward a quantum chemical description of chemical reactions at extreme high pressure. <i>Journal of Computational Chemistry</i> , 2015 , 36, 2246-59	3.5	32
87	Electron correlation and solvation effects. <i>Computational and Theoretical Chemistry</i> , 1991 , 230, 295-312		31
86	Equation of motion for the solvent polarization apparent charges in the polarizable continuum model: application to real-time TDDFT. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 5405-16	2.8	30
85	The decomposition of the SCF interaction energy in hydrogen bonded dimers corrected for basis set superposition errors: An examination of the basis set dependence. <i>International Journal of Quantum Chemistry</i> , 1987 , 32, 227-248	2.1	30
84	Quantum mechanical polarizable continuum model approach to the Kerr effect of pure liquids. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 18706-14	3.4	29
83	Decomposition of the interaction energy between metal cations and water or ammonia with inclusion of counterpoise corrections to the interaction energy terms. <i>Theoretica Chimica Acta</i> , 1989 , 76, 297-313		29
82	Coupled-cluster theory for the polarizable continuum model. III. A response theory for molecules in solution. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 2547-2560	2.1	28
81	Structure versus solvent effects on nonlinear optical properties of push-pull systems: a quantum-mechanical study based on a polarizable continuum model. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 14774-84	2.8	28
80	Synthesis, structure, and electrochemical properties of copper(I) complexes with S/N homoscorpionate and heteroscorpionate ligands. <i>Inorganic Chemistry</i> , 2005 , 44, 4333-45	5.1	28

79	Analytical expressions of the free energy derivatives for molecules in solution. Application to the geometry optimization. <i>International Journal of Quantum Chemistry</i> , 1995 , 56, 695-702	2.1	27
78	Decomposition of the interaction energy with counterpoise corrections to the basis set superposition error for dimers in solution. Method and application to the hydrogen fluoride dimer. <i>Chemical Physics</i> , 1988 , 122, 63-74	2.3	27
77	Modeling Molecular Systems at Extreme Pressure by an Extension of the Polarizable Continuum Model (PCM) Based on the Symmetry-Adapted Cluster-Configuration Interaction (SAC-CI) Method: Confined Electronic Excited States of Furan as a Test Case. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2063-76	6.4	26
76	An ab initio time-dependent Hartree-Fock study of solvent effects on the polarizability and second hyperpolarizability of polyacetylene chains within the polarizable continuum model. <i>Chemical Physics</i> , 1998 , 238, 153-163	2.3	26
75	Synthesis and molecular structure of the dihydrobis(thioxotriazoliny)borato complexes of zinc(II), bismuth(III), and nickel(II). M...H-B interaction studied by Ab initio calculations. <i>Inorganic Chemistry</i> , 2003 , 42, 1769-78	5.1	26
74	On the ab initio geometry optimization of molecular solutes. <i>Journal of Computational Chemistry</i> , 1991 , 12, 301-309	3.5	25
73	Molecular Response Functions for the Polarizable Continuum Model. <i>Springer Briefs in Molecular Science</i> , 2013 ,	0.6	25
72	Solvent Effects on 15N NMR Shielding of 1,2,4,5-Tetrazine and Isomeric Tetrazoles: Continuous Set Gauge Transformation Calculation Using the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 9600-9604	2.8	24
71	Counterpoise corrections to the components of bimolecular energy interactions: An examination of three methods of decomposition. <i>International Journal of Quantum Chemistry</i> , 1986 , 29, 373-378	2.1	24
70	Solvent and vibrational effects on molecular electric properties. Static and dynamic polarizability and hyperpolarizabilities of urea in water. <i>Computational and Theoretical Chemistry</i> , 1998 , 426, 191-198		22
69	A Symmetry adapted tessellation of the GEPOLE surface: applications to molecular properties in solution. <i>Journal of Computational Chemistry</i> , 2001 , 22, 1262-1272	3.5	22
68	Time-dependent variational principle for nonlinear Hamiltonians and its application to molecules in the liquid phase. <i>International Journal of Quantum Chemistry</i> , 1996 , 60, 297-306	2.1	22
67	The cavity electromagnetic field within the polarizable continuum model of solvation. <i>Journal of Chemical Physics</i> , 2014 , 140, 164114	3.9	21
66	Ab initio model to predict NMR shielding tensors for solutes in liquid crystals. <i>International Journal of Quantum Chemistry</i> , 2003 , 93, 121-130	2.1	20
65	Quantum Mechanical Continuum Solvation Models. <i>ChemInform</i> , 2005 , 36, no		19
64	Cavity field effects within a polarizable continuum model of solvation: Application to the calculation of electronic circular dichroism spectra of R-(+)-3-methyl-cyclopentanone. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 826-838	2.1	18
63	Solvent effects on static and dynamic polarizability and hyperpolarizabilities of acetonitrile. <i>Journal of Molecular Structure</i> , 1997 , 436-437, 567-575	3.4	18
62	The cavity electromagnetic field within the polarizable continuum model of solvation: An application to the real-time time dependent density functional theory. <i>Computational and Theoretical Chemistry</i> , 2014 , 1040-1041, 112-119	2	16

61	Noncovalent interactions of medium strength. A revised interpretation and examples of its applications. <i>International Journal of Quantum Chemistry</i> , 1989 , 35, 223-239	2.1	16
60	Optical absorption and fluorescence of PRODAN in solution: Quantum chemical study based on the symmetry-adapted cluster-configuration interaction method. <i>Chemical Physics Letters</i> , 2012 , 552, 53-57	2.5	15
59	Mononuclear and polynuclear copper(I) complexes with a new N,N',S-donor ligand and with structural analogies to the copper thionein core. <i>Inorganic Chemistry</i> , 2007 , 46, 10143-52	5.1	14
58	Self-consistent quantum mechanical model for the description of excitation energy transfers in molecules at interfaces. <i>Journal of Chemical Physics</i> , 2006 , 125, 054710	3.9	14
57	The Cotton-Mouton effect of gaseous N ₂ , CO, CO ₂ , N ₂ O, OCS and CS ₂ : a density functional approach to high-order mixed electric and magnetic properties. <i>Chemical Physics Letters</i> , 2001 , 346, 251-258	2.5	14
56	Neutral organic lewis acids of T-type. <i>International Journal of Quantum Chemistry</i> , 1986 , 29, 527-539	2.1	14
55	A Reappraisal of the Hydrogen Bonding Interaction Obtained by Combining Energy Decomposition Analyses and Counterpoise Corrections. <i>Topics in Molecular Organization and Engineering</i> , 1988 , 507-559		14
54	Second-order Muller-Plesset second derivatives for the polarizable continuum model: theoretical bases and application to solvent effects in electrophilic bromination of ethylene. <i>Theoretical Chemistry Accounts</i> , 2004 , 111, 66-77	1.9	13
53	New developments in the symmetry-adapted algorithm of the Polarizable Continuum Model. <i>Journal of Computational Chemistry</i> , 2004 , 25, 375-85	3.5	13
52	Energy and energy derivatives for molecular solutes: Perspectives of application to hybrid quantum and molecular methods. <i>International Journal of Quantum Chemistry</i> , 1996 , 60, 1165-1178	2.1	13
51	The Extramolecular Electrostatic Potential. An Indicator of the Chemical Reactivity 1991 , 229-268		13
50	Diels-Alder Cycloaddition of Cyclopentadiene and C at the Extreme High Pressure. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 4363-4371	2.8	12
49	Modelling vibrational coupling in DNA oligomers: a computational strategy combining QM and continuum solvation models. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	12
48	Calculation of nonlinear optical susceptibilities of pure liquids within the Polarizable Continuum Model: the effect of the macroscopic nonlinear polarization at the output frequency. <i>Computational and Theoretical Chemistry</i> , 2003 , 633, 209-216		11
47	Equation of motion for the solvent polarization apparent charges in the polarizable continuum model: Application to time-dependent CI. <i>Journal of Chemical Physics</i> , 2017 , 146, 064116	3.9	10
46	Electronic excitation spectra of molecules in solution calculated using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model with perturbative approach. <i>Journal of Chemical Physics</i> , 2014 , 140, 064114	3.9	10
45	Absolute stereochemistry and preferred conformations of urate degradation intermediates from computed and experimental circular dichroism spectra. <i>Organic and Biomolecular Chemistry</i> , 2011 , 9, 5149-55	3.9	10
44	Excitonic splitting in conjugated molecular materials: A quantum mechanical model including interchain interactions and dielectric effects. <i>Physical Review B</i> , 2004 , 70,	3.3	10

43	On the reaction of Ph ₂ PNHPPh ₂ with RNCS (R=Et, Ph, p-NO ₂ C ₆ H ₄): preparation of the zwitterionic ligand EtNHC(S)Ph ₂ P==NPPh ₂ C(S)NEt (HSNS) and the zwitterionic metalate [(SNS)Rh(CO)]. <i>Chemistry - A European Journal</i> , 2005 , 11, 3413-9	4.8	10
42	Non-Bonded Radii of the Atoms Under Compression. <i>ChemPhysChem</i> , 2020 , 21, 2441-2453	3.2	10
41	Insights on the Realgar Crystal Under Pressure from XP-PCM and Periodic Model Calculations. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 8825-8834	2.8	9
40	XP-PCM Calculations of High Pressure Structural and Vibrational Properties of P4S ₃ . <i>Journal of Physical Chemistry A</i> , 2016 , 120, 5136-44	2.8	9
39	Cu(I) dinuclear complexes with tripodal ligands vs monodentate donors: triphenylphosphine, thiourea, and pyridine. A 1H NMR titration study. <i>Inorganic Chemistry</i> , 2006 , 45, 3456-66	5.1	9
38	Infrared linear dichroism in stretched films: Quantum mechanical approach within the polarizable continuum model. <i>International Journal of Quantum Chemistry</i> , 2005 , 104, 716-726	2.1	9
37	Analytical calculation of pressure for confined atomic and molecular systems using the eXtreme-Pressure Polarizable Continuum Model. <i>Journal of Computational Chemistry</i> , 2018 , 39, 2243-2250	3.5	9
36	From Molecular Electrostatic Potentials to Solvation Models and Ending with Biomolecular Photophysical Processes 2010 , 131-170		8
35	Analysis of the interaction energy in the Cu ⁺ -H ₂ O and Cl ⁻ H ₂ O systems, with CP corrections to the BSSE of the separate terms, and MC simulations of the aqueous systems with and without CP corrections. <i>Theoretica Chimica Acta</i> , 1992 , 82, 165-187		8
34	Quantum Chemistry at the High Pressures: The eXtreme Pressure Polarizable Continuum Model (XP-PCM) 2018 , 273-287		8
33	Toward a Quantum-Mechanical Description of 2D-IR Spectra of Solvated Systems: The Vibrational Mode Coupling within A Polarizable Continuum Model. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 4924-4930	2.4	7
32	Low Temperature Absorption Spectrum of LiNiPO ₄ . <i>Physica Status Solidi (B): Basic Research</i> , 1991 , 163, 281-292	1.3	7
31	Molecular interactions in a homogeneous electric field: the (HF) ₂ complex. <i>Theoretica Chimica Acta</i> , 1993 , 85, 167-187		7
30	Relating atomic energy, radius and electronegativity through compression. <i>Chemical Science</i> , 2021 , 12, 2397-2403	9.4	7
29	The Quantum Chemical Study of Chemical Reactions at Extreme High Pressure by Means of the Extreme-Pressure Polarizable Continuum Model. <i>Annual Reports in Computational Chemistry</i> , 2017 , 13, 117-135	1.8	6
28	The virial theorem for the Polarizable Continuum Model. <i>Journal of Chemical Physics</i> , 2014 , 140, 084112	3.9	6
27	SYMMETRY: A computer program for the analysis of the distortions of the MX ₆ (Oh) and MX ₄ (Td) complexes in crystalline environments. <i>Computers & Chemistry</i> , 1994 , 18, 405-411		6
26	Proton and lithium cation interactions with hydrogen sulfide and hydrogen persulfide. <i>Chemical Physics</i> , 1989 , 136, 399-404	2.3	6

25	An open quantum system theory for polarizable continuum models. <i>Journal of Chemical Physics</i> , 2020 , 152, 174114	3.9	5
24	Varying Electronic Configurations in Compressed Atoms: From the Role of the Spatial Extension of Atomic Orbitals to the Change of Electronic Configuration as an Isobaric Transformation. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5047-5056	6.4	5
23	Druckeffekte auf organische Reaktionen in Fluiden – eine neue theoretische Perspektive. <i>Angewandte Chemie</i> , 2017 , 129, 11278-11295	3.6	5
22	A density functional theory study of structural and NMR properties of SNN thiosemicarbazone ligands and their Pd(II) chlorocomplexes. <i>Computational and Theoretical Chemistry</i> , 2003 , 623, 105-119		5
21	Symmetry descent in molecular systems. <i>Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics</i> , 1986 , 8, 1-18		5
20	Quantum optimal control theory for solvated systems. <i>Journal of Chemical Physics</i> , 2019 , 151, 194109	3.9	5
19	Recent Advances in the Coupled-Cluster Analytical Derivatives Theory for Molecules in Solution Described With the Polarizable Continuum Model (PCM). <i>Advances in Quantum Chemistry</i> , 2012 , 1-29	1.4	4
18	Structure and Properties of Molecular Solutes in Electronic Excited States: a Polarizable Continuum Model approach based on the Time-Dependent Density Functional Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008 , 179-208	0.7	3
17	Properties and Spectroscopies		3
16	Beyond the Continuum Approach		3
15	General Response Theory for the Polarizable Continuum Model. <i>Springer Briefs in Molecular Science</i> , 2013 , 23-36	0.6	3
14	High-Pressure-Promoted and Facially Selective Diels-Alder Reactions of Enzymatically Derived -1,2-Dihydrocatechols and Their Acetonide Derivatives: Enantiodivergent Routes to Homochiral and Polyfunctionalized Bicyclo[2.2.2]octenes. <i>Journal of Organic Chemistry</i> , 2020 , 85, 13080-13095	4.2	2
13	Quantum Cluster Theory for the Polarizable Continuum Model (PCM) 2017 , 1517-1556		1
12	The Role of Computational Chemistry in the Experimental Determination of the Dipole Moment of Molecules in Solution. <i>Journal of Computational Chemistry</i> , 2019 , 40, 2309-2317	3.5	1
11	Linear chains of hydrogen molecules under pressure: An extreme-pressure continuum model study. <i>Journal of Chemical Physics</i> , 2019 , 150, 164122	3.9	1
10	Quantum Cluster Theory for the Polarizable Continuum Model (PCM) 2012 , 1043-1066		1
9	How the Molecular Environment Controls Excitation Energy Transfer and Light Harvesting: a Quantum Mechanical Model. <i>AIP Conference Proceedings</i> , 2007 ,	0	1
8	Toward an Understanding of the Pressure Effect on the Intramolecular Vibrational Frequencies of Sulfur Hexafluoride. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 6362-6373	2.8	1

- 7 On the analytical evaluation of the pressure for the extreme-pressure polarizable continuum model (XP-PCM), with application to atoms. *Annual Reports in Computational Chemistry*, **2021**, 17, 3-22 1.8 0
- 6 Properties of Excited States of Molecules in Solution Described with Continuum Solvation Models **2009**, 19-36
- 5 Quantum Cluster Theory for the Polarizable Continuum Model (PCM) **2015**, 1-40
- 4 Modelling vibrational coupling in DNA oligomers: a computational strategy combining QM and continuum solvation models. *Highlights in Theoretical Chemistry*, **2013**, 143-152
- 3 Excitation Energies and Transition Moments from the PCM Linear Response Functions. *Springer Briefs in Molecular Science*, **2013**, 37-45 0.6
- 2 The PCM Model. *Springer Briefs in Molecular Science*, **2013**, 1-11 0.6
- 1 Analytical Derivatives Theory for Molecular Solutes. *Springer Briefs in Molecular Science*, **2013**, 13-22 0.6