Benedito J C Cabral

List of Publications by Year
in descending order

131	2,437	186265	289244
papers	citations	28 h-index	40 g-index

135	135	135	2331
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A first principles approach to the interactions of alkali metal atoms with carbon quantum dots. Computational Materials Science, 2021, 197, 110614.	3.0	1
2	Preferential solvation and optical properties of eumelanin building blocks in binary mixture of methanol and water. Journal of Chemical Physics, 2021, 155, 174504.	3.0	3
3	On the spectral line width broadening for simulation of the two-photon absorption cross-section of para-Nitroaniline in liquid environment. Journal of Molecular Liquids, 2020, 301, 112405.	4.9	7
4	15N NMR Shifts of Eumelanin Building Blocks in Water: A Combined Quantum Mechanics/Statistical Mechanics Approach. Molecules, 2020, 25, 3616.	3.8	3
5	Exploring a near-Hartreeâ€“Fockâ€“Kohnâ€“Sham approach to study electronic properties of azobenzene in interaction with gold: From clusters to the Au(111) surface. Journal of Chemical Physics, 2020, 153, 214701.	3.0	2
6	Liquid water structure from X-ray absorption and emission, NMR shielding and X-ray diffraction. Science China: Physics, Mechanics and Astronomy, 2019, 62, 1.	5.1	5
7	The Kohn-Sham electronic density of states of liquid HCN: Tuning a long-range corrected exchange-correlation functional for predicting electron binding energies. Chemical Physics Letters, 2019, 724, 96-102.	2.6	6
8	Electron Propagator Theory Approach to the Electron Binding Energies of a Prototypical Photo-Switch Molecular System: Azobenzene. Journal of Physical Chemistry A, 2019, 123, 2091-2099.	2.5	11
9	Magnetic properties and core electron binding energies of liquid water. Journal of Chemical Physics, 2018, 148, 044510.	3.0	3
10	Born-Oppenheimer molecular dynamics, hydrogen bond interactions and magnetic properties of liquid hydrogen cyanide. Journal of Molecular Liquids, 2018, 272, 778-786.	4.9	6
11	An electrospray ionization mass spectrometry study of azidoacetic acid/transition metal complexes. Rapid Communications in Mass Spectrometry, 2017, 31, 1001-1013.	1.5	3
12	Electron binding energies and the fundamental gap of a push-pull dye in a polar environment: p-nitroaniline in liquid water. Chemical Physics Letters, 2017, 667, 332-336.	2.6	2
13	Dynamics, magnetic properties, and electron binding energies of H2O2 in water. Journal of Chemical Physics, 2017, 146, 234502.	3.0	4
14	Hydration effects on the electronic properties of eumelanin building blocks. Journal of Chemical Physics, 2016, 145, 084501.	3.0	14
15	Energetics of Radical Formation in Eumelanin Building Blocks: Implications for Understanding Photoprotection Mechanisms in Eumelanin. Journal of Physical Chemistry A, 2016, 120, 10018-10022.	2.5	0
16	A First-Principles Approach to the Dynamics and Electronic Properties of p-Nitroaniline in Water. Journal of Physical Chemistry A, 2016, 120, 3878-3887.	2.5	23
17	Electronic Properties in Supercritical Fluids. Advances in Quantum Chemistry, 2015, , 323-339.	0.8	6
18	Probing Lewis Acidâ€“Base Interactions with Bornâ€“Oppenheimer Molecular Dynamics: The Electronic Absorption Spectrum of p-Nitroaniline in Supercritical CO₂. Journal of Physical Chemistry B, 2015, 119, 8397-8405.	2.6	7

#	Article	IF	Citations
19	A first principles approach to the electronic properties of liquid and supercritical CO2. Journal of Chemical Physics, 2015, 142, 024504.	3.0	15
20	Structure and Electronic Properties of Liquids and Complex Molecular Systems in Solution: Coupling Many-Body Energy Decomposition Schemes to Born-Oppenheimer Molecular Dynamics. Challenges and Advances in Computational Chemistry and Physics, 2015, , 197-217.	0.6	0
21	Ab initio calculation of the electronic absorption spectrum of liquid water. Journal of Chemical Physics, 2014, 140, 164511.	3.0	8
22	Free base phthalocyanine: Influence of thermal effects and dimerization on the electronic absorption spectrum. Chemical Physics Letters, 2014, 595-596, 97-102.	2.6	6
23	Dynamics of complexation and electronic absorption of calix[4]arene-Ar2. Chemical Physics Letters, 2014, 612, 266-272.	2.6	6
24	Structure and electronic properties of a strong dipolar liquid: Bornâ€“Oppenheimer molecular dynamics of liquid hydrogen cyanide. Chemical Physics Letters, 2013, 555, 119-124.	2.6	13
25	Born-Oppenheimer molecular dynamics and electronic properties of chlorophyll-c2 in liquid methanol. Journal of Chemical Physics, 2013, 138, 225102.	3.0	8
26	Ionization of chlorophyll-c2 in liquid methanol. Chemical Physics Letters, 2012, 546, 67-73.	2.6	7
27	Structure and electronic properties of a benzene-water solution. Journal of Chemical Physics, 2012, 136, 014507.	3.0	29
28	Structure and electronic properties of hydrated mesityl oxide: a sequential quantum mechanics/molecular mechanics approach. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
29	Electronic Properties of Hydrogen-Bonded Complexes of Benzene(HCN)_{1â€“4}: Comparison with Benzene(H₂O)_{1â€“4}. Journal of Physical Chemistry A, 2011, 115, 13714-13723.	2.5	5
30	Explicit solvent effects on the visible absorption spectrum of a photosynthetic pigment: Chlorophyll-c2 in methanol. Chemical Physics Letters, 2011, 516, 250-253.	2.6	19
31	Electronic excitation and ionization of hydrogen peroxideâ€“water clusters: Comparison with water clusters. International Journal of Quantum Chemistry, 2011, 111, 1824-1835.	2.0	26
32	Azidoacetone as a complexing agent of transition metals Ni²⁺/Co²⁺ promoted dissociation of the Cï£¿C bond in azidoacetone. Journal of Mass Spectrometry, 2011, 46, 696-704.	1.6	4
33	Electronic properties of a methaneâ€“water solution. Chemical Physics Letters, 2011, 506, 183-189.	2.6	12
34	Electron binding energies of free base porphyrin and magnesium-porphyrin: A sequential Bornâ€“Oppenheimer molecular dynamics/quantum mechanics approach. Computational and Theoretical Chemistry, 2010, 946, 26-32.	1.5	2
35	Electronic properties of liquid hydrogen fluoride: A sequential quantum mechanical/Bornâ€“Oppenheimer molecular dynamics approach. Chemical Physics Letters, 2010, 495, 40-45.	2.6	6
36	Delocalized water and fluoride contributions to Dyson orbitals for electron detachment from the hydrated fluoride anion. Journal of Chemical Physics, 2010, 132, 214507.	3.0	11

#	Article	IF	Citations
37	Ab initio approach to the electronic properties of sodium-ammonia clusters: Comparison with ammonia clusters. Journal of Chemical Physics, 2010, 132, 094307.	3.0	14
38	QM/MM Approaches to the Electronic Spectra of Hydrogen-Bonding Systems with Connection to Many-Body Decomposition Schemes. Advances in Quantum Chemistry, 2010, , 99-144.	0.8	4
39	Dynamic polarizability, Cauchy moments, and the optical absorption spectrum of liquid water: A sequential molecular dynamics/quantum mechanical approach. Journal of Chemical Physics, 2009, 130, 014505.	3.0	24
40	Dipole polarizability and Rayleigh light scattering by the hydrated electron. Chemical Physics Letters, 2009, 481, 73-77.	2.6	11
41	Bornâ˜Oppenheimer Molecular Dynamics of the Hydration of Na⁺ in a Water Cluster. Journal of Physical Chemistry B, 2009, 113, 16151-16158.	2.6	15
42	Energetics of tert-Butoxyl Addition Reaction to Norbornadiene: A Method for Estimating the Ï€-Bond Strength of a Carbonâ˜Carbon Double Bond. Journal of Physical Chemistry A, 2009, 113, 6524-6530.	2.5	4
43	A Simple One-Body Approach to the Calculation of the First Electronic Absorption Band of Water. Journal of Chemical Theory and Computation, 2009, 5, 1829-1837.	5.3	30
44	Electronic Excitation of Cl^{â˜} in Liquid Water and at the Surface of a Cluster: A Sequential Bornâ˜Oppenheimer Molecular Dynamics/Quantum Mechanics Approach. Journal of Physical Chemistry A, 2009, 113, 14684-14690.	2.5	15
45	Study of doubly charged alkaline earth metal and 3â€azidopropionitrile complexes by electrospray ionization mass spectrometry. Rapid Communications in Mass Spectrometry, 2008, 22, 582-590.	1.5	9
46	Bornâ€“Oppenheimer molecular dynamics of phenol in a water cluster. Chemical Physics Letters, 2008, 456, 170-175.	2.6	19
47	Electronic properties of liquid water by sequential molecular dynamics/density functional theory. Chemical Physics Letters, 2008, 460, 466-469.	2.6	17
48	The Changing Hydrogen-Bond Network of Water from the Bulk to the Surface of a Cluster: A Bornâ˜Oppenheimer Molecular Dynamics Study. Journal of the American Chemical Society, 2008, 130, 17955-17960.	13.7	20
49	Câ˜H Bond Dissociation Enthalpies in Norbornane. An Experimental and Computational Study. Organic Letters, 2008, 10, 1613-1616.	4.6	16
50	Energetic Differences between the Five- and Six-Membered Ring Hydrocarbons: Strain Energies in the Parent and Radical Molecules. Journal of Organic Chemistry, 2008, 73, 6213-6223.	3.2	26
51	Electronic properties of liquid ammonia: A sequential molecular dynamics/quantum mechanics approach. Journal of Chemical Physics, 2008, 128, 014506.	3.0	36
52	First principles molecular dynamics of molten NaI: Structure, self-diffusion, polarization effects, and charge transfer. Journal of Chemical Physics, 2007, 127, 094506.	3.0	23
53	Bond-dissociation enthalpies in the gas phase and in organic solvents: Making ends meet. Pure and Applied Chemistry, 2007, 79, 1369-1382.	1.9	16
54	First principles molecular dynamics of molten NaCl. Journal of Chemical Physics, 2007, 126, 124502.	3.0	44

#	Article	IF	Citations
55	Energetics of Câ˜F, Câ˜Cl, Câ˜Br, and Câ˜I Bonds in 2-Haloethanols. Enthalpies of Formation of XCH2CH2OH (X = F, Cl, Br, I) Compounds and of the 2-Hydroxyethyl Radical. Journal of Physical Chemistry A, 2007, 111, 1713-1720.	2.5	29
56	Energetics of the Allyl Group. Journal of Organic Chemistry, 2007, 72, 8770-8779.	3.2	23
57	Electronically excited water aggregates and the adiabatic band gap of water. Journal of Chemical Physics, 2007, 126, 014509.	3.0	20
58	A cost-effective basis-set extrapolation scheme: Application to the energetics of homolytic bond dissociation. Computational and Theoretical Chemistry, 2007, 811, 361-372.	1.5	5
59	Substituent effects on water-assisted proton transfer in [p-XC6H4OHâ€“(H2O)1â€“3]+ clusters. Chemical Physics Letters, 2007, 442, 451-459.	2.6	2
60	Electron binding energies of organic azides: Greenâ€™s function and density functional theory versus Hartreeâ€“Fock calculations. Chemical Physics Letters, 2007, 448, 280-286.	2.6	5
61	Complexation of transition metals by 3-azidopropionitrile. An electrospray ionization mass spectrometry study. Journal of the American Society for Mass Spectrometry, 2007, 18, 453-465.	2.8	11
62	Conformational and Orientational Guidance of the Analgesic Dipeptide Kyotorphin Induced by Lipidic Membranes:â€‰ Putative Correlation toward Receptor Docking. Journal of Physical Chemistry B, 2006, 110, 3385-3394.	2.6	17
63	Enthalpy of Formation of the Cyclopentadienyl Radical:Â Photoacoustic Calorimetry and ab Initio Studies. Journal of Physical Chemistry A, 2006, 110, 5130-5134.	2.5	22
64	Reply to comment on â€˜The enthalpy of the Oâ€“H bond homolytic dissociation: Basis-set extrapolated density functional theory and coupled cluster calculationsâ€™. Chemical Physics Letters, 2006, 417, 570-572.	2.6	8
65	Photochemistry of AgClâ€“water clusters: Comparison with Clâ˜â€“water clusters. Chemical Physics Letters, 2006, 419, 340-345.	2.6	15
66	The enthalpy of formation of the pentane-2,4-dionate radical: A complete basis set approach. Chemical Physics Letters, 2006, 419, 486-491.	2.6	9
67	Sâ€“H bond dissociation enthalpies: The importance of a complete basis set approach. Chemical Physics Letters, 2006, 421, 504-507.	2.6	24
68	Electron binding energies of water clusters: Implications for the electronic properties of liquid water. Chemical Physics Letters, 2006, 429, 129-135.	2.6	28
69	Carbonâ€“hydrogen bond dissociation enthalpies in ethers: a theoretical study. Computational and Theoretical Chemistry, 2005, 719, 109-114.	1.5	25
70	Oxygenâ€“oxygen bond dissociation enthalpies of di-tert-butyl peroxide and di-trifluoromethyl peroxide. Computational and Theoretical Chemistry, 2005, 729, 223-227.	1.5	14
71	The enthalpy of the Oâ€“H bond homolytic dissociation: Basis-set extrapolated density functional theory and coupled cluster calculations. Chemical Physics Letters, 2005, 406, 300-305.	2.6	39
72	Electronic polarization in liquid acetonitrile: A sequential Monte Carlo/quantum mechanics investigation. Chemical Physics Letters, 2005, 407, 13-17.	2.6	48

#	Article	IF	Citations
73	The vibrational structure of the OH radical in solid argon: A transfer-matrix path-integral approach. International Journal of Quantum Chemistry, 2005, 103, 610-616.	2.0	1
74	Polarization effects and charge separation in AgCl-water clusters. Journal of Chemical Physics, 2005, 122, 044316.	3.0	26
75	The Kohn-Sham density of states and band gap of water: From small clusters to liquid water. Journal of Chemical Physics, 2005, 123, 054510.	3.0	52
76	Energetics of Hydroxybenzoic Acids and of the Corresponding Carboxyphenoxyl Radicals. Intramolecular Hydrogen Bonding in 2-Hydroxybenzoic Acid. Journal of Physical Chemistry A, 2005, 109, 9700-9708.	2.5	33
77	The density of states and band gap of liquid water by sequential Monte Carlo/Quantum mechanics calculations. Brazilian Journal of Physics, 2004, 34, 42-47.	1.4	17
78	Homolytic dissociation in hydrogen-bonding liquids: energetics of the phenol O?H bond in methanol and the water O?H bond in water. Theoretical Chemistry Accounts, 2004, 112, 282.	1.4	7
79	Reaction ofpara-Hydroxy-Substituted Diphenylmethanes withtert-Butoxy Radical. ChemPhysChem, 2004, 5, 1217-1221.	2.1	12
80	Structural, energetic, and electronic properties of (CH3CN)2â€“8 clusters by density functional theory. Computational and Theoretical Chemistry, 2004, 673, 155-164.	1.5	31
81	Charge separation and charge transfer to solvent in NaClâ€“water clusters. Chemical Physics Letters, 2004, 399, 200-205.	2.6	17
82	Can larger dipoles solvate less? soluteâ€“solvent hydrogen bond and the differential solvation of phenol and phenoxy. Chemical Physics Letters, 2004, 399, 534-538.	2.6	18
83	Oâ€“H Bond dissociation enthalpies in hydroxyphenols. A time-resolved photoacoustic calorimetry and quantum chemistry study. Physical Chemistry Chemical Physics, 2004, 6, 2109-2118.	2.8	24
84	Filipin Orientation Revealed by Linear Dichroism. Implication for a Model of Action. Journal of the American Chemical Society, 2004, 126, 5396-5402.	13.7	21
85	Energetics of Intramolecular Hydrogen Bonding in Di-substituted Benzenes by the orthoâ^'para Method. Journal of Physical Chemistry A, 2004, 108, 10834-10843.	2.5	94
86	First-principles molecular dynamics of liquid rubidium at low density. Journal of Non-Crystalline Solids, 2004, 347, 100-105.	3.1	7
87	Electronic polarization of liquid water: converged Monte Carlo-quantum mechanics results for the multipole moments. Chemical Physics Letters, 2003, 369, 345-353.	2.6	67
88	Solvent Effects on the Energetics of the Phenol Oâ^'H Bond:Â Differential Solvation of Phenol and Phenoxy Radical in Benzene and Acetonitrile. Journal of Physical Chemistry A, 2003, 107, 9197-9207.	2.5	36
89	Differential Hydration of Phenol and Phenoxy Radical and the Energetics of the Phenol Oâ^'H Bond in Solution. Journal of Physical Chemistry B, 2003, 107, 4304-4310.	2.6	35
90	Binding energy, structure, and vibrational spectra of (HCl)2â€“6 and (HF)2â€“10 clusters by density functional theory. Journal of Chemical Physics, 2003, 118, 1272-1281.	3.0	46

#	Article	IF	Citations
91	The hydration of the OH radical: Microsolvation modeling and statistical mechanics simulation. Journal of Chemical Physics, 2003, 119, 7344-7355.	3.0	80
92	Sâ^'H Bond Dissociation Enthalpies in Thiophenols:Â A Time-Resolved Photoacoustic Calorimetry and Quantum Chemistry Studyâ€. Journal of Physical Chemistry A, 2002, 106, 9883-9889.	2.5	75
93	Energetics of the Câ^'Cl Bond in CH3CH(Cl)COOH. Enthalpy of Formation of (S)-(â^')-2-Chloropropionic Acid and of the 1-Carboxyethyl Radicalâ€,â€¡. Journal of Physical Chemistry A, 2002, 106, 9855-9861.	2.5	7
94	Complexation of Calix[4]arene With Alkali Metal Cations: Conformational Binding Selectivity and Cation-Ï€ Driven Inclusion. Supramolecular Chemistry, 2002, 14, 57-66.	1.2	42
95	Metastability and weak mixing in classical long-range many-rotator systems. Physical Review E, 2002, 66, 065101.	2.1	36
96	Ab initio molecular dynamics of liquid Kâ€“Tl. Journal of Non-Crystalline Solids, 2002, 312-314, 69-73.	3.1	1
97	Phenol O-H bond dissociation energy in water clusters. International Journal of Quantum Chemistry, 2002, 86, 297-304.	2.0	28
98	Hydrogen bonding and the dipole moment of hydrofluorocarbons by density functional theory. Physical Chemistry Chemical Physics, 2001, 3, 4200-4207.	2.8	47
99	Fluids of strongly interacting dipoles: Monte Carlo sampling using Tsallis statistics. Physica A: Statistical Mechanics and Its Applications, 2001, 295, 234-241.	2.6	1
100	Structure and conformational equilibrium of thiacalix[4]arene by density functional theory. Computational and Theoretical Chemistry, 2001, 549, 253-260.	1.5	59
101	Structure of polydisperse dipolar hard-sphere fluids. Journal of Chemical Physics, 2000, 112, 4351-4356.	3.0	31
102	Thermochemical Properties and Structure of Phenolâ^'(H2O)1-6 and Phenoxyâ^'(H2O)1-4 by Density Functional Theory. Journal of Physical Chemistry A, 2000, 104, 6062-6068.	2.5	39
103	Homocoordination preference in NaCs and LiNa liquid alloys by first principles molecular dynamics. Journal of Chemical Physics, 1999, 111, 5067-5072.	3.0	10
104	Structure, Conformational Equilibrium, and Proton Affinity of Calix[4]arene by Density Functional Theory. Journal of Physical Chemistry A, 1999, 103, 9080-9085.	2.5	58
105	First principles molecular dynamics of a liquid Liâ€“Na alloy. Computational and Theoretical Chemistry, 1999, 463, 145-149.	1.5	3
106	Ab initio and density functional theory calculations of molecular structure and vibrational spectrum of ethyl azidoacetate. Computational and Theoretical Chemistry, 1999, 469, 55-61.	1.5	2
107	Substituent effects on the O-H bond dissociation enthalpies in phenolic compounds: agreements and controversies. Pure and Applied Chemistry, 1999, 71, 1249-1256.	1.9	58
108	Theoretical calculations of the molecular properties of a CFC substitute: CHCl2CF3 (HCFC123). Computational and Theoretical Chemistry, 1998, 452, 117-124.	1.5	2

#	Article	IF	Citations
109	Hydrogen bonding and conformational equilibrium in p-tert-butyldihomooxacalix[4]arene. Computational and Theoretical Chemistry, 1998, 455, 23-32.	1.5	15
110	Experimental and theoretical proton affinity of limonene. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1427-1430.	1.7	25
111	Ab initio and density functional study of azidoacetone. Computational and Theoretical Chemistry, 1997, 397, 223-230.	1.5	5
112	Condensed-phase effects on the conformational equilibrium of ethylene glycol. International Journal of Quantum Chemistry, 1996, 60, 1651-1660.	2.0	6
113	Density-functional and density-functional reaction field calculations of the molecular properties of phenol. Chemical Physics Letters, 1996, 258, 436-444.	2.6	19
114	First principles molecular dynamics simulation of liquid rubidium. Computational and Theoretical Chemistry, 1995, 330, 273-277.	1.5	0
115	Molecular properties of 2-azidoethanol and 2-chloroethyl azide. A theoretical study. Computational and Theoretical Chemistry, 1995, 339, 143-151.	1.5	8
116	Density functional study of molecular properties of hydrazoic acid and methyl azide. Computational and Theoretical Chemistry, 1995, 343, 31-41.	1.5	16
117	First-principles molecular dynamics of liquid cesium and rubidium. Physical Review B, 1995, 51, 872-877.	3.2	23
118	Vapor-Liquid Equilibrium and Structure of Methyl Iodide Liquid. The Journal of Physical Chemistry, 1995, 99, 5180-5186.	2.9	18
119	Dissociation mechanisms of energy-selected chlorobutane ions: Experiment and theory. Organic Mass Spectrometry, 1993, 28, 1229-1237.	1.3	4
120	Monte Carlo simulation of the methylchloride liquid-vapour interface. Journal of Physics Condensed Matter, 1993, 5, 1919-1934.	1.8	4
121	Improved propagators for the path integral study of quantum systems. Journal of Chemical Physics, 1993, 98, 3300-3305.	3.0	2
122	UVPES of some aliphatic azides Part III. Journal of Molecular Structure, 1991, 249, 181-188.	3.6	10
123	A Monte Carlo and transfer-matrix grid path-integral study of the vibrational structure of Br2 in solid argon. Chemical Physics Letters, 1991, 184, 53-60.	2.6	10
124	Ab initio study of the conformational equilibrium of ethylene glycol. Theoretica Chimica Acta, 1991, 78, 271-280.	0.8	33
125	The structure of molten CsAu: ab initio and Monte Carlo study. Journal of Physics Condensed Matter, 1991, 3, 5615-5620.	1.8	7
126	UVPES of some aliphatic azides. Part II. Journal of Molecular Structure, 1990, 220, 315-319.	3.6	9

#	Article	IF	Citations
127	A Monte Carlo simulation study of a polarizable liquid: Influence of the electrostatic induction on its thermodynamic and structural properties. Journal of Chemical Physics, 1987, 86, 1467-1473.	3.0	21
128	Influence of dispersion forces on the electronic structure of a solvated molecule. Chemical Physics Letters, 1986, 125, 495-499.	2.6	50
129	Conformational equilibrium of 1,2â€dichloroethane in methylchloride. A Monte Carlo simulation of the differential gaucheâ€“anti solvation. Journal of Chemical Physics, 1985, 83, 3083-3094.	3.0	41
130	A Monte Carlo study of electrostatic solvation energies in molecular liquids. Chemical Physics Letters, 1982, 93, 157-161.	2.6	9
131	New basis set for molecular calculations. II. A CNDO study of electric dipole moments and electronic valence population on AH and AB systems using the modified Slater orbitals. Journal of Physics B: Atomic and Molecular Physics, 1980, 13, 211-216.	1.6	0