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394	On the Calculation of Infrared Intensities in Solution within the Polarizable Continuum Model. 2000 , 104, 9874-9879		77
393	Ab Initio Study of the Electronic Excited States in 4-(N,N-Dimethylamino)benzonitrile with Inclusion of Solvent Effects: The Internal Charge Transfer Process. 2000 , 122, 10621-10630		88
392	Fast Evaluation of Geometries and Properties of Excited Molecules in Solution: A Tamm-Dancoff Model with Application to 4-Dimethylaminobenzonitrile. 2000 , 104, 5631-5637		484
391	Solvent Effects on Nuclear Shieldings: "Continuum or Discrete Solvation Models To Treat Hydrogen Bond and Polarity Effects?". 2001 , 105, 7287-7296		105
390	Calculation of Optical Rotation Using Density Functional Theory. 2001 , 105, 5356-5371		324
389	Theoretical Approach to the Calculation of Vibrational Raman Spectra in Solution within the Polarizable Continuum Model. 2001 , 105, 8310-8316		49
388	Theoretical Study of the Photophysics of Adenine in Solution: "Tautomerism, Deactivation Mechanisms, and Comparison with the 2-Aminopurine Fluorescent Isomer. 2001 , 105, 4749-4757		117

- 387 Solvent Effects on *trans/gauche* Conformational Equilibria of Substituted Chloroethanes: a Polarizable Continuum Model Study. **2001**, 105, 10807-10815 35
- 386 Theoretical Study of Guanine from Gas Phase to Aqueous Solution: Role of Tautomerism and Its Implications in Absorption and Emission Spectra. **2001**, 105, 7126-7134 76
- 385 Correlation between molecular structure and helicity of induced chiral nematics in terms of short-range and electrostatic-induction interactions. The case of chiral biphenyls. **2001**, 123, 7842-51 72
- 384 Effects of Induction Interactions on the Orientational Order of Solutes in Liquid Crystals. **2001**, 105, 2837-2849 17
- 383 Comment on Reaction field treatment of charge penetration [J. Chem. Phys. 112, 5558 (2000)]. **2001**, 114, 4744 141
- 382 Energy correction to simulation of volume polarization in reaction field theory. **2002**, 116, 10129-10138 35
- 381 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 CCl₄ Solution. **2002**, 106, 12331-12339 79
- 380 A molecular based continuum approach for the dielectric permittivity of liquids and liquid crystals. **2002**, 117, 2397-2414 4
- 379 Hydrogen bond versus polar effects: an ab initio analysis on n → π* absorption spectra and N nuclear shieldings of diazines in solution. **2002**, 124, 1506-15 91
- 378 Polarizable Continuum Model (PCM) Calculations of Solvent Effects on Optical Rotations of Chiral Molecules. **2002**, 106, 6102-6113 494
- 377 An integrated effective fragment polarizable continuum approach to solvation: Theory and application to glycine. **2002**, 116, 5023 114
- 376 Solvent effects on glycine. I. A supermolecule modeling of tautomerization via intramolecular proton transfer. **2003**, 24, 1789-802 62
- 375 A density functional theory study of structural and NMR properties of SNN thiosemicarbazone ligands and their Pd(II) chlorocomplexes. **2003**, 623, 105-119 5
- 374 Quantum mechanical calculations coupled with a dynamical continuum model for the description of dielectric relaxation: Time dependent Stokes shift of coumarin C153 in polar solvents. **2003**, 108, 21-46 33
- 373 Molecular Models of Orientational Order. **2003**, 241-258 1
- 372 Prediction of Solvent Effects on Vibrational Absorption Intensities and Raman Activities in Solution within the Polarizable Continuum Model: A Study on Push-Pull Molecules. **2003**, 107, 10261-10271 11
- 371 The Cotton-Mouton effect of furan and its homologues in the gas phase, for the pure liquids and in solution. **2003**, 118, 10712-10724 36
- 370 The modeling and simulation of the liquid phase. **2003**, 10, 271-375 1

369	A polarizable continuum model for molecules at diffuse interfaces. 2004 , 120, 3893-907	62
368	Excitonic splitting in conjugated molecular materials: A quantum mechanical model including interchain interactions and dielectric effects. 2004 , 70,	10
367	Intermolecular interactions in solution: elucidating the influence of the solvent. 2004 , 120, 2802-13	39
366	Quantum-Mechanical Continuum Solvation Study of the Polarizability of Halides at the Water/Air Interface. 2004 , 108, 13796-13806	34
365	New developments in the symmetry-adapted algorithm of the Polarizable Continuum Model. 2004 , 25, 375-85	13
364	Solvent effects on glycine II. Water-assisted tautomerization. 2004 , 25, 690-703	58
363	Solvation response in water: a study based on molecular dynamics simulations and quantum mechanical calculations. 2005 , 117, 85-92	5
362	Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. 2005 , 727, 29-40	74
361	Building cavities in a fluid of spherical or rod-like particles: a contribution to the solvation free energy in isotropic and anisotropic polarizable continuum model. 2005 , 26, 1096-105	17
360	The effects of solvation in the theoretical spectra of cationic dyes. 2005 , 113, 274-280	67
359	Infrared linear dichroism in stretched films: Quantum mechanical approach within the polarizable continuum model. 2005 , 104, 716-726	9
358	Effect of the environment on vibrational infrared and circular dichroism spectra of (s)-proline. 2005 , 104, 744-757	26
357	Accurate prediction of electron-paramagnetic-resonance tensors for spin probes dissolved in liquid crystals. 2005 , 123, 194909	11
356	Two-photon absorption in solution by means of time-dependent density-functional theory and the polarizable continuum model. 2005 , 122, 244104	97
355	Gauge-origin-independent magnetizabilities of solvated molecules using the polarizable continuum model. 2005 , 123, 204104	3
354	Second-harmonic generation of solvated molecules using multiconfigurational self-consistent-field quadratic response theory and the polarizable continuum model. 2005 , 123, 144117	41
353	Induced Charge Computation Method. 2005 , 19-43	3
352	The reorganization energy of azurin in bulk solution and in the electrochemical scanning tunneling microscopy setup. 2005 , 109, 3423-30	35

351	How to model solvation of peptides? Insights from a quantum-mechanical and molecular dynamics study of N-methylacetamide. 1. Geometries, infrared, and ultraviolet spectra in water. 2005 , 109, 9818-29	83
350	A combined theoretical and experimental approach to determining order parameters of solutes in liquid crystals from ¹³ C NMR data. 2005 , 109, 2584-90	20
349	Birefringences: A Challenge for Both Theory and Experiment. 2005 , 143-184	26
348	Quantum mechanical polarizable continuum model approach to the Kerr effect of pure liquids. 2005 , 109, 18706-14	29
347	How to model solvation of peptides? Insights from a quantum mechanical and molecular dynamics study of N-methylacetamide. 2. ¹⁵ N and ¹⁷ O nuclear shielding in water and in acetone. 2005 , 109, 9830-8	36
346	Conformation and orientation of tetraalanine in a lyotropic liquid crystal studied by nuclear magnetic resonance. 2005 , 109, 21102-9	7
345	Quantum mechanical continuum solvation models. 2005 , 105, 2999-3093	11786
344	Polarizable continuum model study of solvent effects on electronic circular dichroism parameters. 2005 , 122, 024106	57
343	Toward a molecular scale interpretation of excitation energy transfer in solvated bichromophoric systems. 2005 , 127, 16733-44	72
342	Environmental effects on the spectroscopic properties of gallic acid: a combined classical and quantum mechanical study. 2005 , 109, 1933-43	63
341	The effect of protein dielectric coefficient on the ionic selectivity of a calcium channel. 2006 , 125, 34901	85
340	Regioselectivity in lithiation of 1-methylpyrazole: experimental, density functional theory and multinuclear NMR study. 2006 , 4, 1261-7	12
339	Solvation of N ₃ ⁻ at the water surface: the polarizable continuum model approach. 2006 , 110, 11361-8	13
338	On the origin of the stereoselectivity in the alkylation of oxazolopiperidone enolates. 2006 , 128, 6581-8	15
337	Solvation of coumarin 153 in supercritical fluoroform. 2006 , 110, 4953-62	32
336	Combined density functional/polarizable continuum model study of magnetochiral birefringence: can theory and experiment be brought to agreement?. 2006 , 125, 234105	23
335	Density-functional-theory study of the electric-field-induced second harmonic generation (EFISHG) of push-pull phenylpolyenes in solution. 2006 , 425, 267-272	96
334	Theoretical predictions for occurrence of charge transfer complex within the two synthesized bichromophores considering the role of their spacers in interactions with the orbitals of the redox centers. 2006 , 428, 213-219	2

333	Structural characterization of agmatine at physiological conditions. 2006 , 17, 163-175	18
332	DFT Calculation of Deuterium Quadrupolar Tensor in Crystal Anthracene. 2006 , 116, 711-717	4
331	Solvation of monovalent anions in acetonitrile and N,N-dimethylformamide: Parameterization of the IEF-PCM model. 2006 , 331, 142-158	99
330	Nature of base stacking: reference quantum-chemical stacking energies in ten unique B-DNA base-pair steps. 2006 , 12, 2854-65	204
329	Dispersion and repulsion contributions to the solvation free energy: comparison of quantum mechanical and classical approaches in the polarizable continuum model. 2006 , 27, 1769-80	44
328	Order parameters of alpha,omega-diphenylpolyenes in a nematic liquid crystal from an integrated computational and ¹³ C NMR spectroscopic approach. 2006 , 125, 174904	1
327	Self-consistent quantum mechanical model for the description of excitation energy transfers in molecules at interfaces. 2006 , 125, 054710	14
326	Parallelization of the integral equation formulation of the polarizable continuum model for higher-order response functions. 2006 , 125, 154112	10
325	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. 2007 , 126, 124114	74
324	An ab initio investigation of the Buckingham birefringence of furan, thiophene, and selenophene in cyclohexane solution. 2007 , 127, 164321	12
323	Conformational analysis of L-prolines in water. 2007 , 111, 14034-42	48
322	Properties and structure of aromatic ester solvents. 2007 , 111, 4417-31	9
321	How solvent controls electronic energy transfer and light harvesting: toward a quantum-mechanical description of reaction field and screening effects. 2007 , 111, 13253-65	102
320	Degenerate four-wave mixing in solution by cubic response theory and the polarizable continuum model. 2007 , 111, 8965-73	15
319	Towards a molecular scale interpretation of excitation energy transfer in solvated bichromophoric systems. II. The through-bond contribution. 2007 , 111, 853-63	43
318	Computational study on the properties and structure of methyl lactate. 2007 , 111, 4671-83	24
317	Computational study of anion solvation in nitrobenzene. 2007 , 436, 362-367	10
316	Spectroscopic properties and photophysics of the synthesized compound 5-nitro-benzo[b]thiophene-2-carboxylic acid in non-polar/polar media and in the presence of TiO ₂ nanoparticles. 2007 , 127, 541-551	

315	DFT calculation and Raman excitation profile studies of benzophenone molecule. 2007 , 44, 331-342	28
314	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. 2007 , 117, 793-803	1
313	Cationic dye dimers: a theoretical study. 2007 , 118, 305-314	14
312	Phenolic esters with potential anticancer activity--the structural variable. 2007 , 13, 865-77	18
311	An IEF-PCM study of solvent effects on the Faraday ($\{B\}$) term of MCD. 2008 , 119, 231-244	28
310	Solvent effects on the nitrogen NMR shielding and nuclear quadrupole coupling constants in 1-methyltriazoles. 2008 , 460, 129-136	15
309	Solvation of monovalent anions in formamide and methanol: Parameterization of the IEF-PCM model. 2008 , 344, 101-113	7
308	Theoretical study of structure and electronic properties of cyano-substituted pyrroles. 2008 , 353, 177-184	11
307	Measurements and predictive models for the N-methyl-2-pyrrolidone/water/methanol system. 2008 , 112, 11361-73	38
306	Does Förster theory predict the rate of electronic energy transfer for a model dyad at low temperature?. 2008 , 112, 3759-66	60
305	Structure-directed reversion in the pi-facial stereoselective alkylation of chiral bicyclic lactams. 2008 , 73, 7756-63	12
304	Response of Scalar Fields and Hydrogen Bonding to Excited-State Molecular Solvation of Carbonyl Compounds. 2008 , 4, 578-85	8
303	Claisen rearrangement of aliphatic allyl vinyl ethers in the presence of copper(II) bisoxazoline. 2008 , 73, 4800-9	12
302	Modeling the solvation of peptides. The case of (s)-N-acetylproline amide in liquid water. 2008 , 112, 3441-50	25
301	An efficient implementation for determining volume polarization in self-consistent reaction field theory. 2008 , 129, 194109	16
300	The initial and final states of electron and energy transfer processes: diabaticization as motivated by system-solvent interactions. 2009 , 130, 234102	117
299	Structure versus solvent effects on nonlinear optical properties of push-pull systems: a quantum-mechanical study based on a polarizable continuum model. 2009 , 113, 14774-84	28
298	Theoretical approaches to the calculation of Raman optical activity spectra. 2009 , 21 Suppl 1, E54-67	90

297	Wavelet formulation of the polarizable continuum model. 2010 , 31, 1469-77	13
296	Antioxidant phenolic esters with potential anticancer activity: solution equilibria studied by Raman spectroscopy. 2009 , 40, 80-85	15
295	DFT and electrochemical studies on nortriptyline oxidation sites. 2009 , 15, 945-52	11
294	Wavelet BEM on molecular surfaces: parametrization and implementation. 2009 , 86, 1-22	15
293	Hydrogen bonding and solution state structure of salicylaldehyde-4-phenylthiosemicarbazone: A combined experimental and theoretical study. 2009 , 919, 66-71	20
292	First-Principles Determination of Molecular Conformations of Indolizidine (-)-235B' in Solution. 2009 , 124, 269-278	3
291	Density functional and spectroscopic studies of nitrogen inversion in substituted dizocilpines. 2009 , 22, 607-612	1
290	Theoretical study of structural and optical properties of regioregular head-to-tail oligo (3-n-octylthiophene) and related star molecules. 2009 , 910, 104-111	7
289	Quantum cluster theory for the polarizable continuum model. I. The CCSD level with analytical first and second derivatives. 2009 , 131, 164104	69
288	Pyrrolidone Derivatives in Water Solution: An Experimental and Theoretical Perspective. 2009 , 48, 1036-1050	31
287	Nonplasmonic Metal Particles as Excitation Energy Transfer Acceptors: an Unexpected Efficiency Revealed by Quantum Mechanics. 2009 , 113, 16364-16370	19
286	Jones and magnetoelectric birefringence of pure substances [A computational study. 2009 , 87, 1352-1361	5
285	Fluorescence Enhancement of Chromophores Close to Metal Nanoparticles. Optimal Setup Revealed by the Polarizable Continuum Model. 2009 , 113, 121-133	123
284	Microsolvation of methyl hydrogen peroxide: ab initio quantum chemical approach. 2009 , 131, 054310	10
283	Quantum mechanical and NMR studies of ring puckering and cis/trans-rotameric interconversion in prolines and hydroxyprolines. 2009 , 113, 10858-65	29
282	Insights into the ethyl lactate + water mixed solvent. 2009 , 113, 14257-69	38
281	The green solvent ethyl lactate: an experimental and theoretical characterization. 2009 , 11, 65-78	166
280	Probing weak non-covalent interactions in solution and solid states with designed molecules. 2009 , 11, 97-100	21

279	Structures and properties of electronically excited chromophores in solution from the polarizable continuum model coupled to the time-dependent density functional theory. 2009 , 113, 3009-20	158
278	Theoretical study on the molecular and electronic properties of some substances used for diabetes mellitus treatment. 2010 , 16, 799-804	12
277	Steady-state and time-resolved spectroscopic investigations on intramolecular electron transfer processes within a synthesized methoxynaphthalene dyad by using a nematic liquid crystal medium. 2010 , 130, 932-940	1
276	Photoinduced processes of 3-substituted 6-fluoro-1,4-dihydro-4-oxoquinoline derivatives: A theoretical and spectroscopic study. 2010 , 211, 47-58	9
275	A comparative molecular dynamics study on the complexation of alkali metal cations by a poly-ethylene-glycol type podand in water and in dichloromethane. 2010 , 946, 77-82	8
274	Study of the solvent effect on the enthalpies of homolytic and heterolytic N-H bond cleavage in p-phenylenediamine and tetracyano-p-phenylenediamine. 2010 , 952, 25-30	220
273	Theoretical study of tautomerization and isomerization of methylamino- and phenylamino-substituted cyclic azaphospholines, oxaphospholines and thiaphospholines in gas and aqueous phases. 2010 , 962, 101-107	5
272	On the geometrical structure and spectral properties of pyrene monomer and sterically constrained intramolecular pyrene dimers. 2010 , 377, 123-131	7
271	Excited-state polarizabilities of solvated molecules using cubic response theory and the polarizable continuum model. 2010 , 132, 024107	8
270	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. 2010 , 133, 024104	70
269	Superexchange-mediated electronic energy transfer in a model dyad. 2010 , 12, 7378-85	31
268	Continuous surface charge polarizable continuum models of solvation. I. General formalism. 2010 , 132, 114110	1701
267	Mechanism of water oxidation by single-site ruthenium complex catalysts. 2010 , 132, 1545-57	424
266	On the Calculation of Vibrational Frequencies for Molecules in Solution Beyond the Harmonic Approximation. 2010 , 6, 1660-9	51
265	A variational formulation of the polarizable continuum model. 2010 , 133, 014106	103
264	Light-induced oxidation of unsaturated lipids as sensitized by flavins. 2010 , 114, 5583-93	47
263	Experimental verification of force fields for molecular dynamics simulations using Gly-Pro-Gly-Gly. 2010 , 114, 12358-75	39
262	Continuum Solvation Models: What Else Can We Learn from Them?. 2010 , 1, 1666-1674	116

261	Classical valence bond approach by modern methods. 2011 , 111, 7557-93	190
260	Polarizable Force Fields and Polarizable Continuum Model: A Fluctuating Charges/PCM Approach. 1. Theory and Implementation. 2011 , 7, 3711-24	126
259	Integrated NMR and computational study of push-pull NLO probes: interplay of solvent and structural effects. 2011 , 115, 10035-44	10
258	Excitation energies in solution: the fully polarizable QM/MM/PCM method. 2011 , 115, 3027-37	108
257	Self-Consistent Field and Polarizable Continuum Model: A New Strategy of Solution for the Coupled Equations. 2011 , 7, 610-7	28
256	Isolation of a metastable geometrical isomer of a hexacoordinated dihydrophosphate: elucidation of its enhanced reactivity in umpolung of a hydrogen atom of water. 2011 , 50, 9083-9	8
255	On the enthalpies of homolytic and heterolytic S-H bond cleavage in para and meta substituted thiophenols. 2011 , 967, 273-283	27
254	DFT/B3LYP study of the solvent effect on the reaction enthalpies of homolytic and heterolytic OH bond cleavage in mono-substituted chromans. 2011 , 978, 16-28	29
253	A DFT study of the properties of substituted pyrrolidines and phospholanes in gas and in aqueous phase. 2011 , 978, 143-151	2
252	Modulating spectroelectrochemical properties of [Ni(salen)] polymeric films at molecular level. 2011 , 161, 680-691	24
251	Study of dimethoxyethane/ethanol solutions. 2011 , 115, 8864-74	21
250	Response Function Theory Computational Approaches to Linear and Nonlinear Optical Spectroscopy. 2011 , 77-135	21
249	Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a β -extended TTF derivative. 2011 , 13, 11965-75	14
248	Modeling of the functionalization of single-wall carbon nanotubes towards its solubilization in an aqueous medium. 2011 , 61, 381-388	12
247	On analytical derivatives for geometry optimization in the polarizable continuum model. <i>Journal of Mathematical Chemistry</i> , 2011 , 49, 1928-1936	2.1 2
246	Wavelet BEM on molecular surfaces: solvent excluded surfaces. 2011 , 92, 335-364	18
245	Spectroscopic investigations on Naphthol and Tetrahydronaphthol. A theoretical approach. 2011 , 78, 624-8	3
244	Anodic oxidation of selenadiazoloquinolones in alkaline media. 2011 , 49, 168-74	3

243	Symmetric versus asymmetric discretization of the integral equations in polarizable continuum solvation models. 2011 , 509, 77-87	58
242	Theoretical and spectroscopic study of ethyl 1,4-dihydro-4-oxoquinoline-3-carboxylate and its 6-fluoro and 8-nitro derivatives in neutral and radical anion forms. 2011 , 994, 61-69	10
241	Towards an accurate description of anharmonic infrared spectra in solution within the polarizable continuum model: reaction field, cavity field and nonequilibrium effects. 2011 , 135, 104505	45
240	Nonequilibrium solvation for vertical photoemission and photoabsorption processes using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model. 2011 , 134, 104109	50
239	Catalytic activity of halohydrin dehalogenases towards spiroepoxides. 2012 , 10, 5063-72	38
238	Conformational behaviour of antioxidant chromones. A vibrational spectroscopy study. 2012 , 63, 325-337	13
237	Modeling ultrafast solvated electronic dynamics using time-dependent density functional theory and polarizable continuum model. 2012 , 116, 1884-90	25
236	Oxidation mechanism of methionine by HO \cdot radical: a theoretical study. 2012 , 116, 5349-54	9
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234	A Novel Approach for Deriving Force Field Torsion Angle Parameters Accounting for Conformation-Dependent Solvation Effects. 2012 , 8, 3232-42	23
233	How amidoximate binds the uranyl cation. 2012 , 51, 3855-9	137
232	Stereoelectronic interactions and the one-bond C-F coupling constant in sevoflurane. 2012 , 116, 1677-82	26
231	State-of-the-art and challenges in theoretical simulations of heterogeneous catalysis at the microscopic level. 2012 , 2, 2405	34
230	Simultaneous gauche and anomeric effects in β -substituted sulfoxides. 2012 , 77, 7607-11	17
229	Three routes to nickel(II) salicylaldehyde 4-phenyl and 4-methylthiosemicarbazonato complexes: mechanochemical, electrochemical and conventional approach. 2012 , 14, 3039	15
228	Linear Response Theory and Electronic Transition Energies for a Fully Polarizable QM/Classical Hamiltonian. 2012 , 8, 4153-65	100
227	Excited states and electronic spectra of annulated dinuclear free-base phthalocyanines: a theoretical study on near-infrared-absorbing dyes. 2012 , 136, 114304	9
226	Recent Advances in the Coupled-Cluster Analytical Derivatives Theory for Molecules in Solution Described With the Polarizable Continuum Model (PCM). 2012 , 1-29	4

225	VBEFP: a valence bond approach that incorporates effective fragment potential method. 2012 , 116, 1846-53	12
224	Structures in solutions from joint experimental-computational analysis: applications to cyclic molecules and studies of noncovalent interactions. 2012 , 116, 1093-109	9
223	Assessment of DFT Exchange-Correlation Functionals for Evaluating the Multipolar Contributions to the Quadratic Nonlinear Optical Responses of Small Reference Molecules. 2012 , 8, 2044-52	42
222	Theoretical Investigation on the Solubilization in Water of Functionalized Single-Wall Carbon Nanotubes. 2012 , 2012, 1-6	22
221	Polarizable continuum model. 2012 , 2, 386-404	480
220	Revised self-consistent continuum solvation in electronic-structure calculations. 2012 , 136, 064102	293
219	Recent advances in wave function-based methods of molecular-property calculations. 2012 , 112, 543-631	453
218	Synthesis and Conformational Analysis of Methyl N-Alanyl-1 α -aminoferrocene-1-carboxylate. 2012 , 2012, 1810-1822	15
217	An Integrated approach (thermodynamic, structural, and computational) to the study of complexation of alkali-metal cations by a lower-rim calix[4]arene amide derivative in acetonitrile. 2012 , 51, 6264-78	27
216	Theoretical insights into the mechanism of carbon monoxide (CO) release from CO-releasing molecules. 2012 , 18, 9267-75	21
215	3-Fluoro-N-methyl-D-aspartic acid (3F-NMDA) stereoisomers as conformational probes for exploring agonist binding at NMDA receptors. 2012 , 18, 8813-9	31
214	Diastereomer configurations from joint experimental-computational analysis. 2012 , 77, 6290-5	10
213	Modelling zwitterions in solution: 3-fluoro- β -aminobutyric acid (3F-GABA). 2012 , 18, 184-95	11
212	Balancing the atomic waistline: Isodensity-based scrf radii for main-group elements and transition metals. 2013 , 113, 975-984	42
211	Ab initio nonorthogonal valence bond methods. 2013 , 3, 56-68	16
210	Three Polymorphic Forms of a Monomeric Mo(VI) Complex: Building Blocks for Two Metal-Organic Supramolecular Isomers. Intermolecular Interactions and Ligand Substituent Effects. 2013 , 13, 3773-3784	31
209	On the radical scavenging activity of isoflavones: thermodynamics of O-H bond cleavage. 2013 , 15, 10895-903	69
208	Experimental and computational study of the complexation of adamantyl glycosides with β -cyclodextrin. 2013 , 69, 8051-8063	9

207	Quantum chemical and experimental study of 1,2,4-trihydroxy-para-menthane. 2013 , 1049, 494-501	3
206	Conformational analysis of 1-chloro- and 1-bromo-2-propanol. 2013 , 117, 10980-4	4
205	The triflic acid-mediated cyclization reactions of N-cinnamoyl-1-naphthylamines. 2013 , 78, 10938-46	13
204	Partial molar volume, Jones-Dole coefficient, and limiting molar isentropic compressibility of sodium ibuprofen in water and its hydration number and hydration free energy. 2013 , 566, 124-129	19
203	Donor Abilities of Heterocyclic Neutral Lewis Bases in a Nickel(II) Salicylaldehyde 4-Phenylthiosemicarbazonato Coordination Environment. 2013 , 2013, 563-571	3
202	Critical Evaluation of Implicit Solvent Models for Predicting Aqueous Oxidation Potentials of Neutral Organic Compounds. 2013 , 9, 5046-58	80
201	Potential of polyphenols from an aqueous extract of apple peel as inhibitors of free radicals: An experimental and computational study. 2013 , 1035, 61-68	11
200	A generalized G-SFED continuum solvation free energy calculation model. 2013 , 110, E662-7	8
199	Computational Spectroscopy of Large Systems in Solution: The DFTB/PCM and TD-DFTB/PCM Approach. 2013 , 9, 2052-71	41
198	The anomeric effect on the basis of natural bond orbital analysis. 2013 , 11, 2885-90	62
197	Conformational analysis and intramolecular interactions in aminofluorobenzoic acids. 2013 , 117, 1659-64	10
196	Fast Domain Decomposition Algorithm for Continuum Solvation Models: Energy and First Derivatives. 2013 , 9, 3637-48	64
195	Mechanism elucidation of the cis-trans isomerization of an azole ruthenium-nitrosyl complex and its osmium counterpart. 2013 , 52, 6260-72	23
194	Circular dichroism and optical rotation of lactamide and 2-aminopropanol in aqueous solution. 2013 , 117, 5136-47	15
193	Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle. 2013 , 139, 024105	13
192	Gradient Models in Molecular Biophysics: Progress, Challenges, Opportunities. 2013 , 22, 169-184	10
191	Theoretical study of the electronic excitations of free-base porphyrin-Ar ₂ van der Waals complexes. 2013 , 139, 074303	3
190	THEORETICAL STUDY OF THE SUBSTITUENT EFFECTS ON THE REACTION ENTHALPIES OF THE ANTIOXIDANT MECHANISMS OF STOBADINE DERIVATIVES IN THE GAS-PHASE AND WATER. 2013 , 12, 1250116	13

189	Conformational analysis and intramolecular interactions in monosubstituted phenylboranes and phenylboronic acids. 2013 , 9, 1127-34	6
188	Computer Simulations of Prebiotic Systems. 2014 ,	5
187	Electronic excitation spectra of molecules in solution calculated using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model with perturbative approach. 2014 , 140, 064114	10
186	Motional timescale predictions by molecular dynamics simulations: case study using proline and hydroxyproline sidechain dynamics. 2014 , 82, 195-215	128
185	Investigation of oxidation attack sites in sterols: Thermodynamics of hydrogen atom transfer. 2014 , 1038, 26-32	11
184	C longitudinal relaxation time measurements and DFT-GIAO NMR computations for two ammonium ions of a tetraazamacrocyclic system. 2014 , 78, 299-310	6
183	Density, viscosity and ultrasonic velocity studies of aqueous solutions of sodium salicylate and its hydration free energy. 2014 , 52, 7-16	7
182	1?-Acetylferrocene amino acid esters and amides. A simple model for parallel α -helical peptides. 2014 , 70, 2330-2342	5
181	The gauche effect is governed by internal hydrogen bond in 2-amino-2-methyl-propanol. 2014 , 1072, 203-207	4
180	Reaction enthalpies of OH bonds splitting-off in flavonoids: The role of non-polar and polar solvent. 2014 , 1050, 31-38	44
179	Quantum mechanics/molecular mechanics modeling of photoelectron spectra: the carbon 1s core-electron binding energies of ethanol-water solutions. 2014 , 118, 13217-25	12
178	An efficient computational scheme for electronic excitation spectra of molecules in solution using the symmetry-adapted cluster-configuration interaction method: the accuracy of excitation energies and intuitive charge-transfer indices. 2014 , 141, 154104	10
177	A Novel Series of CoIII(salen-type) Complexes Containing a Seven-Membered Metallacycle: Synthesis, Structural Characterization and Factors Affecting the Metallacyclization Rate. 2014 , 33, 909-920	6
176	Solvation at Surfaces and Interfaces: A Quantum-Mechanical/Continuum Approach Including Nonelectrostatic Contributions. 2014 , 118, 4715-4725	18
175	Facile tuning of the aggregation-induced emission wavelength in a common framework of a cyclometalated iridium(III) complex: micellar encapsulated probe in cellular imaging. 2014 , 2, 5615-5628	46
174	Study of the chelating properties of Ge(OH) ₂ functionality as metal binding group for Zn ²⁺ cation in simplified protease-like environments: a DFT analysis. 2014 , 20, 2430	2
173	Physicochemical and biological properties of luteolin-7-O- β -D-glucoside (cynaroside) isolated from <i>Anthriscus sylvestris</i> (L.) Hoffm.. 2014 , 145, 1307-1318	19
172	Cationic Half-Sandwich Iron(II) and Iron(III) Complexes with N-Heterocyclic Carbene Ligands. 2014 , 33, 5670-5677	29

171	Computational study of the structure-free radical scavenging relationship of procyanidins. 2014 , 161, 155-61	26
170	Electrochemical Solvent Reorganization Energies in the Framework of the Polarizable Continuum Model. 2014 , 10, 2091-102	32
169	Modeling environment effects on pigment site energies: Frozen density embedding with fully quantum-chemical protein densities. 2014 , 1040-1041, 347-359	18
168	Substituent effect on supramolecular motifs in series of succinimide polycyclic keto derivatives □ Spectroscopic, theoretical and crystallographic studies. 2014 , 1074, 695-702	3
167	Quantum, classical, and hybrid QM/MM calculations in solution: general implementation of the ddCOSMO linear scaling strategy. 2014 , 141, 184108	37
166	Modeling solvation effects in real-space and real-time within density functional approaches. 2015 , 143, 144111	9
165	Electronic excitation of molecules in solution calculated using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model. 2015 ,	3
164	DFT-Aided Vibrational Circular Dichroism Spectroscopy Study of (-)-S-cotinine. 2015 , 16, 1416-27	5
163	Theoretical insight into the mechanism of gold(I)-catalyzed rearrangement of 2-propargyl 2H-azirines to pyridines. 2015 , 80, 3547-55	23
162	Modeling of single-walled carbon nanotubes functionalized with carboxylic and amide groups towards its solubilization in water. 2015 , 212, 592-596	23
161	Wavelet formulation of the polarizable continuum model. II. Use of piecewise bilinear boundary elements. 2015 , 17, 31566-81	9
160	Calculation of Electrochemical Reorganization Energies for Redox Molecules at Self-Assembled Monolayer Modified Electrodes. 2015 , 6, 1-5	11
159	Antioxidant properties of xanthones extracted from the pericarp of <i>Garcinia mangostana</i> (Mangosteen): A theoretical study. 2015 , 625, 30-35	40
158	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. 2015 , 11, 2063-76	26
157	Building blocks for bioinspired electrets: molecular-level approach to materials for energy and electronics. 2015 , 87, 779-792	21
156	Highly enantioselective construction of tertiary thioethers and alcohols phosphine-catalyzed asymmetric addition reactions of 5-thiazol-4-ones and 5-oxazol-4-ones: scope and mechanistic understandings. 2015 , 6, 4912-4922	113
155	Synthesis and Optical Properties of Imidazole- and Benzimidazole-Based Fused π-Conjugated Compounds: Influence of Substituent, Counteranion, and π-Conjugated System. 2015 , 80, 7172-83	18
154	Theoretical calculation of the maximum absorption wavelength for Cyanidin molecules with several methodologies. 2015 , 1067, 129-134	19

153	Importance of asparagine on the conformational stability and chemical reactivity of selected anti-inflammatory peptides. 2015 , 457, 180-187	2
152	Asymmetric binuclear Ni(II) and Cu(II) Schiff base metallopolymers. 2015 , 5, 39495-39504	3
151	Combined experimental and computational investigation of the absorption spectra of E- and Z-cinnamic acids in solution: The peculiarity of Z-cinnamics. 2015 , 148, 128-135	13
150	Computational Spectroscopy in Solution: Methods and Models for Investigating Complex Systems. 2015 , 447-517	1
149	The conjugates of ferrocene-1,1'-diamine and amino acids. A novel synthetic approach and conformational analysis. 2015 , 44, 16405-20	14
148	Conformational properties of chiral tobacco alkaloids by DFT calculations and vibrational circular dichroism: (-)-S-anabasine. 2015 , 60, 169-79	4
147	Solvent effect on the anodic oxidation of tannic acids: EPR/UV-Vis spectroelectrochemical and DFT theoretical study. 2015 , 19, 2533-2544	5
146	Electrochemically driven molecular rotors based on ferrocene-1,1'-diyl-bisphosphinic acids. 2015 , 51, 645-664	3
145	Highly selective recognition of tryptophan in water by a poorly water-soluble scandium compound. 2015 , 56, 5557-5560	
144	Prospects for the Computational Design of BipyridineN,N'-Dioxide Catalysts for Asymmetric Propargylation Reactions. 2015 , 5, 272-280	41
143	Hydration Effect on Amide I Infrared Bands in Water: An Interpretation Based on an Interaction Energy Decomposition Scheme. 2015 , 119, 9056-67	14
142	Vibrational circular dichroism and theoretical study of the conformational equilibrium in (-)-S-nicotine. 2015 , 16, 342-52	9
141	Synthesis and Conformational Study of Bioconjugates Derived from 1-Acetyl-1'-aminoferrocene and α -Amino Acids. 2015 , 2015, 112-123	7
140	Four-component relativistic calculations in solution with the polarizable continuum model of solvation: theory, implementation, and application to the group 16 dihydrides H ₂ X (X = O, S, Se, Te, Po). 2015 , 119, 5061-77	13
139	Theoretical study of the substituent effects on O-H BDE of trans-resveratrol derivatives in water and benzene: NBO analysis of intramolecular hydrogen bonds. 2015 , 26, 47-59	2
138	Intra- and intermolecular hydrogen bonding in acetylacetone and benzoylacetone derived enamionone derivatives. 2015 , 1079, 243-249	18
137	The Intersection of NO and HS: Persulfides Generate NO from Nitrite through Polysulfide Formation. 2016 , 55, 12618-12625	28
136	Synthesis and Electropolymerization of Bis(phenylthieno[3,2-b]thiophenes) (4,4'-dinonyl-2,2'-bithiazole) co-monomer. 2016 , 222, 1592-1603	11

135	Combining the GW formalism with the polarizable continuum model: A state-specific non-equilibrium approach. 2016 , 144, 164106	30
134	A polarizable continuum model for molecules at spherical diffuse interfaces. 2016 , 144, 124103	9
133	Density functional theory studies of conformational stabilities and rotational barriers of 2- and 3-thiophenecarboxaldehydes. 2016 , 57, 1545-1553	10
132	Deprotonation of flavonoids severely alters the thermodynamics of the hydrogen atom transfer. 2016 , 1085, 7-17	28
131	Antioxidant activities of [60]fullerene derivatives from chalcone, flavone and flavanone: A ONIOM approach via H-atom and electron transfer mechanism. 2016 , 652, 56-61	5
130	Electronic excitation and ionization behavior of N-hydroxypyridine-2(1H)-thione and its deprotonated anion in a polarizable medium studied using quantum chemical computations. 2016 , 135, 1	3
129	Functionalization of fullerene via the Bingel reaction with trichlorocarbanions: an ONIOM approach. 2016 , 22, 113	4
128	Novel Stannatrane N(CHCMeO)(CMeCHO)SnO-t-Bu and Related Oligonuclear Tin(IV) Oxoclusters. Two Isomers in One Crystal. 2016 , 55, 10218-10228	21
127	Computational Studies of Environmental Effects and Their Interplay With Experiment. 2016 , 203-241	2
126	Clay/Organic Hybrid Films Exhibiting Reversible Fluorescent Color Switching Induced by Swelling and Drying of a Clay Mineral. 2016 , 120, 23813-23822	11
125	Divergent Synthesis of Three Classes of Antifungal Amphiphilic Kanamycin Derivatives. 2016 , 81, 10651-10663	14
124	One-pot synthesis and theoretical calculation for trifluoromethylated pyrrolizidines by 1,3-dipolar cycloaddition with azomethine ylides and trifluoromethyl acrylamides. 2016 , 189, 22-32	11
123	Proton-Coupled Electron Transfer in a Strongly Coupled Photosystem II-Inspired Chromophore-Imidazole-Phenol Complex: Stepwise Oxidation and Concerted Reduction. 2016 , 138, 11536-49	46
122	Ferrocene in oil/water interfaces: An electrochemical approach. 2016 , 212, 195-200	1
121	Design of Organocatalysts for Asymmetric Propargylations through Computational Screening. 2016 , 6, 7948-7955	51
120	Quantum chemistry calculations of technetium and rhenium compounds with application in radiopharmacy: review. 2016 , 6, 107127-107140	7
119	A new discretization for the polarizable continuum model within the domain decomposition paradigm. 2016 , 144, 054101	17
118	The nitrogen inversion in fused isoxazolidinyl derivatives of substituted uracil: synthesis, NMR and computational analysis. 2016 , 27, 1265-1278	7

117	Heterodinuclear Ni(ii) and Cu(ii) Schiff base complexes and their activity in oxygen reduction. 2016 , 45, 14725-33		7
116	Electrochemical Electron Transfer and Proton-Coupled Electron Transfer: Effects of Double Layer and Ionic Environment on Solvent Reorganization Energies. 2016 , 12, 2917-25		24
115	DFT study of the hydrolysis reaction in atranes and ocanes: the influence of transannular bonding. 2016 , 22, 3		6
114	Theoretical investigation of the solubilization of COOH-functionalized single wall carbon nanotubes in water. 2016 , 215, 780-786		27
113	Association of Catechin Molecules in Water: Quantitative Binding Study and Complex Structure Analysis. 2016 , 79, 66-73		17
112	The structure of tagetitoxin. 2016 , 14, 238-45		6
111	Thermodynamic study of vitamin B6 antioxidant potential. 2016 , 1077, 32-38		16
110	Conformations of Flavan-3-ols in Water: Analysis Using Density Functional Theory. 2017 , 80, 319-327		6
109	Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. 2017 , 13, 3185-3197		733
108	Helically Chiral Peptides That Contain Ferrocene-1,1'-diamine Scaffolds as a Turn Inducer. 2017 , 23, 10372-10395		5
107	Zero interval limit perturbation expansion for the spectral entities of Hilbert-Schmidt operators combined with most dominant spectral component extraction: convergence and confirmative implementations. <i>Journal of Mathematical Chemistry</i> , 2017 , 55, 1278-1300	2.1	1
106	Solvent Effects on Optical Rotation: On the Balance between Hydrogen Bonding and Shifts in Dihedral Angles. 2017 , 121, 4765-4777		7
105	DFT Study of the Molecular Structure, Conformational Preference, HOMO, LUMO, and Vibrational Analysis of 2-, and 3-Furoyl Chloride. 2017 , 46, 741-758		13
104	Synthesis and Characterization of Dithienothiophene, Bithiazole and Thiophene Containing Polymer. 2017 , 227, 435-446		10
103	Effect of Orbital Interactions between Vicinal Bonds and between Hydroxy Groups on the Conformational Stabilities of 1,2-Ethenediol and 2,3-Butanediols. 2017 , 121, 8484-8494		6
102	Synthesis and Optical Properties of Excited-State Intramolecular Proton Transfer Active EConjugated Benzimidazole Compounds: Influence of Structural Rigidification by Ring Fusion. 2017 , 82, 12173-12180		23
101	Construction of 6-thioguanine and 6-mercaptopurine carriers based on cyclodextrins and gold nanoparticles. 2017 , 177, 22-31		20
100	Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution. 2017 , 16, 1415-1423		10

99	Solubility of amide functionalized single wall carbon nanotubes: A quantum mechanical study. 2017 , 242, 1208-1214	22
98	Computation of forces arising from the polarizable continuum model within the domain-decomposition paradigm. 2017 , 147, 224108	8
97	Four-Component Relativistic Density Functional Calculations of EPR Parameters for Model Complexes of Tungstoenzymes. 2017 , 121, 9106-9117	4
96	Zero interval limit perturbation expansion for the spectral entities of Hilbert-Schmidt operators combined with most dominant spectral component extraction: formulation and certain technicalities. <i>Journal of Mathematical Chemistry</i> , 2017 , 55, 1253-1277	2.1 2
95	Open-ended formulation of self-consistent field response theory with the polarizable continuum model for solvation. 2016 , 19, 366-379	3
94	Four-component relativistic density functional theory with the polarisable continuum model: application to EPR parameters and paramagnetic NMR shifts. 2017 , 115, 214-227	15
93	Synthesis and Conformational Study of Monosubstituted Aminoferrocene-Based Peptides Bearing Homo- and Heterochiral Pro-Ala Sequences. 2017 , 2017, 306-317	4
92	Photodynamic Efficiency of Xanthene Dyes and Their Phototoxicity against a Carcinoma Cell Line: A Computational and Experimental Study. 2017 , 2017, 1-9	20
91	A DFT Study of Structural and Bonding Properties of Complexes Obtained from First-Row Transition Metal Chelation by 3-Alkyl-4-phenylacetylamino-4,5-dihydro-1H-1,2,4-triazol-5-one and Its Derivatives. 2017 , 2017, 5237865	10
90	On Autonomy Imposition in Zero Interval Limit Perturbation Expansion for the Spectral Entities of Hilbert-Schmidt Integral Operators. 2017 , 5, 2	4
89	Time dependent-density functional theory (TD-DFT) and experimental studies of UV-Visible spectra and cyclic voltammetry for Cu(II) complex with Et ₂ DTC. 2018 , 1157, 463-468	3
88	Atomic charges for conformationally rich molecules obtained through a modified principal component regression. 2018 , 20, 2890-2903	1
87	Quantum chemistry in arbitrary dielectric environments: Theory and implementation of nonequilibrium Poisson boundary conditions and application to compute vertical ionization energies at the air/water interface. 2018 , 148, 222834	20
86	Computational Prediction of H and C NMR Chemical Shifts for Protonated Alkylpyrroles: Electron Correlation and Not Solvation is the Salvation. 2019 , 20, 78-91	9
85	Impact of Ligand Substitutions on Multielectron Redox Properties of Fe Complexes Supported by Nitrogenous Chelates. 2018 , 3, 14766-14778	6
84	Relativistic heavy atom effect on the P NMR parameters of phosphine chalcogenides. Part 1. Chemical shifts. 2018 , 56, 1061-1073	9
83	Experimental and theoretical studies of a greener catalytic system for saturated hydrocarbon chlorination composed by trichloroisocyanuric acid and a copper(II) compound. 2018 , 562, 150-158	1
82	Calculation of N and P NMR Chemical Shifts of Azoles, Phospholes, and Phosphazoles: A Gateway to Higher Accuracy at Less Computational Cost. 2018 , 122, 6746-6759	8

81	Toward a Predictive Understanding of Phosphine-Catalyzed [3 + 2] Annulation of Allenates with Acrylate or Imine. 2018 , 83, 9729-9740	15
80	Computational Investigation into the Ni(SeNHC(CN)) and Ni(SNHC(CN)) Complexes as Potential Catalysts for Hydrogen Production. 2019 , 123, 7822-7827	2
79	Quantum Calculations in Solution of Energies, Structures, and Properties with a Domain Decomposition Polarizable Continuum Model. 2019 , 15, 6061-6073	8
78	Quantum Chemical Study on the High-Pressure Effect for [4 + 4] Retrocycloaddition of Anthracene Cyclophane Photodimer. 2019 , 123, 4493-4501	4
77	Corrosion inhibition of X80 steel in simulated acid wash solution using glutathione and its blends: Experimental and theoretical studies. 2019 , 578, 123597	19
76	Molecular Hydration of Carbonic Acid: Ab Initio Quantum Chemical and Density Functional Theory Investigation. 2019 , 123, 5504-5516	6
75	Ten-membered rings as key interaction motifs in folding of desmuramyl di-, tri-, and tetrapeptides. 2019 , 30, 743-754	1
74	Influence and Substituent Effects on the HOMO-LUMO Energy Gap and Stokes Shift in Ru Mono-Diimine Derivatives. 2019 , 1195, 620-631	3
73	Computationally-assisted discovery and structure elucidation of natural products. 2019 , 73, 687-695	11
72	Conformational Stabilities, Rotational Barriers, and Vibrational Spectra of 2-Pyrrolicarboxaldehyde and 3-Pyrrolicarboxaldehyde Calculated Using Density Functional Theory. 2019 , 60, 186-197	5
71	Electrochemical kinetics, molecular dynamics, adsorption and anticorrosion behavior of melatonin biomolecule on steel surface in acidic medium. 2019 , 129, 42-53	26
70	Theoretical insight into the photodeactivation pathway of the tetradentate Pt (II) complex with different inductive substituents. 2019 , 33, e4879	3
69	A Domain Decomposition Method for the Poisson-Boltzmann Solvation Models. 2019 , 41, B320-B350	7
68	Nonequilibrium Solvent Polarization Effects in Real-Time Electronic Dynamics of Solute Molecules Subject to Time-Dependent Electric Fields: A New Feature of the Polarizable Continuum Model. 2019 , 15, 2306-2319	8
67	Efficient implementation of the analytical second derivatives of hartree-fock and hybrid DFT energies within the framework of the conductor-like polarizable continuum model. 2019 , 40, 1816-1828	14
66	Multimodal switching of a redox-active macrocycle. 2019 , 10, 1007	13
65	Parametric representation of molecular surfaces. 2019 , 119, e25695	1
64	Complex Structures of Monoglucosylrutin with ent-Gallocatechin-3- O-gallate and Epigallocatechin-3- O-gallate in Aqueous Solutions and the Mechanism of Color Change Induced by Complexation. 2019 , 82, 2-8	3

63	Catalyst-Inspired Charge Carriers for High Energy Density Redox Flow Batteries. 2019 , 6,	6
62	PCMSolver: An open-source library for solvation modeling. 2019 , 119, e25685	20
61	Solvation thermodynamics of neutral and charged solutes using the solvation-layer interface condition continuum dielectric model. 2019 , 119, e25771	1
60	Long-range relativistic heavy atom effect on ¹ H NMR chemical shifts of selenium- and tellurium-containing compounds. 2019 , 119, e25809	11
59	Intrinsically smooth discretisation of Connolly's solvent-excluded molecular surface. 2020 , 118, e1644384	9
58	Benzothiazole merocyanine dyes as middle pH optical sensors. 2020 , 176, 108193	13
57	Solvent dependence of the stereoselectivity in bipyridine N,N'-dioxide catalyzed allylation of aromatic aldehydes: A computational perspective. 2020 , 483, 110712	1
56	Mechanism of Copigmentation of Monoglucosylrutin with Caffeine. 2020 , 68, 323-331	1
55	Effect of the Solute Cavity on the Solvation Energy and its Derivatives within the Framework of the Gaussian Charge Scheme. 2020 , 41, 922-939	33
54	Anti-corrosion behaviour of 4(p-tolyldiazenyl)-2-((E)-(p-tolylimino)methyl)phenol on mild steel in 1M H ₂ SO ₄ : Experimental and theoretical studies. 2020 , 7, e00256	3
53	Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. 2020 , 60, 249-258	8
52	Inhibition of erosion corrosion of pipework steel in descaling solution using 5-hydroxytryptamine-based additives: Empirical and computational studies. 2020 , 1204, 127562	11
51	Density Functional Theory Investigation of As(III) S-Adenosylmethionine Methyltransferase. 2020 , 5, 21000-21006	
50	Antioxidant action of deprotonated flavonoids: Thermodynamics of sequential proton-loss electron-transfer. 2020 , 180, 112528	25
49	Expanding the potential of redox carriers for flow battery applications. 2020 , 8, 17808-17816	2
48	Simulating Plasmon Resonances of Gold Nanoparticles with Bipyramidal Shapes by Boundary Element Methods. 2020 , 16, 3807-3815	9
47	NMR absolute shielding scales and nuclear magnetic dipole moments of transition metal nuclei. 2020 , 22, 7065-7076	5
46	Antioxidant Properties of Lapachol and Its Derivatives and Their Ability to Chelate Iron (II) Cation: DFT and QTAIM Studies. 2020 , 2020, 2103239	2

45	Experimental, adsorption, quantum chemical and molecular dynamics simulation studies on the corrosion inhibition performance of Vincamine on J55 steel in acidic medium. 2021 , 1227, 129533	10
44	Guest-Host Interactions in Symmetrical Carboxy Heptamethine Cyanine Dyes-Titanium Dioxide Systems: Synthesis, Theoretical Calculations, Aggregation Properties, and Application in Dye-Sensitized Solar Cells. 2021 , 2021, 1-17	
43	A fast direct solver for nonlocal operators in wavelet coordinates. 2021 , 428, 110056	0
42	Dielectric continuum methods for quantum chemistry. 2021 , 11, e1519	31
41	Computational investigation of the reaction of nickel-bis(dithiolene) and nickel-bis(diselenolene) complexes with OH. 2021 , 99, 346-353	
40	A Density Functional Theory Study of Optical Rotation in Some Aziridine and Oxirane Derivatives. 2021 , 22, 764-774	0
39	Role of Hydrogen Bonds in Formation of Co-amorphous Valsartan/Nicotinamide Compositions of High Solubility and Durability with Anti-hypertension and Anti-COVID-19 Potential. 2021 , 18, 1970-1984	6
38	The best density functional theory functional for the prediction of H and C chemical shifts of protonated alkyppyroles. 2021 , 42, 1248-1262	2
37	Describing ground and excited state potential energy surfaces for molecular photoswitches using coupled cluster models. 2021 , 42, 1419-1429	1
36	LayerPCM: An implicit scheme for dielectric screening from layered substrates. 2021 , 154, 224114	3
35	Computational Chemistry of Pyrrolidone and Caprolactam Based Materials. 1365-1458	
34	Mechanistic Insights into Promoted Hydrolysis of Phosphoester Bonds by MoOCl(DMF). 2021 , 60, 11177-111913	
33	New Insights on the Interaction of Phenanthroline Based Ligands and Metal Complexes and Polyoxometalates with Duplex DNA and G-Quadruplexes. 2021 , 26,	4
32	Multireference Perturbation Theory Combined with PCM and RISM Solvation Models: A Benchmark Study for Chemical Energetics. 2021 , 125, 8324-8336	0
31	Contrasting roles of bond orbital interactions contributing to conformational stabilities of flavan-3-ol structures. 2021 , 1203, 113362	
30	Reaction-based machine learning representations for predicting the enantioselectivity of organocatalysts. 2021 , 12, 6879-6889	15
29	Prediction of the standard potentials for one-electron oxidation of ,,,' tetrasubstituted -phenylenediamines by calculation. 2021 , 23, 20340-20351	1
28	Informing saccharide structural NMR studies with density functional theory calculations. 2015 , 1273, 289-331	14

27	Molecular Surface Decomposition Using Graphical Modeling. 2008 , 197-201	5
26	Thermodynamics of primary antioxidant action of flavonols in polar solvents. 2019 , 12, 108-118	2
25	Adsorption of Mercury(II) Chloride and Carbon Dioxide on Graphene/Calcium Oxide (0 0 1). 2016 , 26, 298-305	19
24	Thermodynamics of radical scavenging effect of deprotonated isoflavones in aqueous solution. 2022 , 345, 117861	6
23	Solvent Effects and Chemical Reactivity. 2009 ,	1
22	Liquid-Phase Simulation: Theory and Numerics of Hybrid Quantum-Mechanical/Classical Approaches. 2015 , 811-817	
21	Asymmetric Construction of Tertiary/Secondary Carbon-Phosphorus Bonds via Bifunctional Phosphonium Salt Catalyzed 1,6-Addition. 14168-14180	1
20	DFT STUDY OF THE STRUCTURE, CONFORMATIONAL PROFILE AND THE VIBRATIONAL ANALYSIS OF 2-FURANCARBOETHIALDEHYDE AND 3-FURANCARBOETHIALDEHYDE. 2021 , 62, 1485-1497	
19	Theoretical Investigation of Glycine Micro-Solvated. Energy and NMR Spin Spin Coupling Constants Calculations. 2021 , 3, 41	
18	Theoretical Modeling of Redox Potentials of Biomolecules.. 2022 , 27,	2
17	Investigation of oxygen influence to the optical properties of tirapazamine.. 2022 , 28, 96	
16	Ligand-induced donor state destabilisation - a new route to panchromatically absorbing Cu(I) complexes.. 2022 ,	0
15	Implicit Solvation Methods for Catalysis at Electrified Interfaces.. 2021 ,	11
14	A promising strategy for increasing phosphorescent quantum yield: The ligand 10-cyclic chelate of the tetradentate Pt(II) complex. 2022 , 36,	1
13	Optimal control for semilinear integrodifferential evolution equations in Banach spaces. 1-7	
12	Thermochemistry of antioxidant action of isoflavones and their deprotonated forms in aqueous solution: hydrogen or electron transfer?. 2022 , 15, 29-35	
11	Synthesis, solid-state, solution, and theoretical characterization of an [In-cage]candium-NOTA complex.	
10	Quantification of the Strength of [Noncovalent Interactions in Molecular Balances using Density Functional Methods.	

- 9 Implicit and explicit solvent models have opposite effects on radiation damage rate constant for thymine. **2022**, 245-265
- 8 Detection of catechins using a fluorescent molecule and its application toward the evaluation of astringent intensity.
- 7 Photophysics of Anionic Bis(4H-imidazolato)Cu(I) Complexes.
- 6 Quantum Simulation of Molecules in Solution.
- 5 Modeling the electronic structure of organic materials: a solid-state physicist's perspective. **2023**, 6, 012001
- 4 Turning enol* emission of SBOH via restricting twisted intramolecular charge transfer behavior by pressure. **2023**, 294, 122551
- 3 Neutral, Heteroleptic [Cu(I)(PPh₃)₂(4 H -imidazolato)] Complexes: Ligand Exchange Reactivity, Redox Properties, Excited-State Dynamics.
- 2 Computation of entropy values for non-electrolyte solute molecules in solution based on semi-empirical corrections to a polarized continuum model. **2023**, 25, 8082-8089
- 1 Solvent Induced Proton Polarization within the Nuclear-Electronic Orbital Framework. **2023**, 14, 2990-2995