

# Ivelina Georgieva

## List of Publications by Year in descending order

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64  
papers

1,045  
citations

394286

19  
h-index

477173

29  
g-index

64  
all docs

64  
docs citations

64  
times ranked

1472  
citing authors

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 1  | Structural characterisation, Hirshfeld surfaces, DSC, periodic DFT modeling, vibrational and optical study of heptylenediammonium pentachlorobismuthate H <sub>3</sub> N(CH <sub>2</sub> ) <sub>7</sub> NH <sub>3</sub> BiCl <sub>5</sub> . <i>Journal of Solid State Chemistry</i> , 2022, 306, 122805.                         | 1.4 | 10        |
| 2  | Spectroscopic and photophysical properties of [Eu(Phen) <sub>2</sub> ] <sub>3</sub> (X <sup>+</sup> ; Cl <sup>-</sup> , NO <sub>3</sub> <sup>-</sup> ) complexes, incorporated into SiO <sub>2</sub> -based Matrices: Theoretical study. <i>Materials Today: Proceedings</i> , 2022, 61, 1292-1299.                              | 0.9 | 1         |
| 3  | Effect of urea on arrangement of novel Mg(II) perhenate crystal structures and their optical properties: Experimental and theoretical insight. <i>Journal of Solid State Chemistry</i> , 2022, 312, 123263.  | 1.4 | 2         |
| 4  | Crystalline adducts of urea with magnesium iodide. <i>Journal of Molecular Structure</i> , 2021, 1224, 129009.   | 1.8 | 2         |
| 5  | Phenanthroline chromophore as efficient antenna for Tb <sup>3+</sup> green luminescence: A theoretical study. <i>Dyes and Pigments</i> , 2021, 185, 108890.  | 2.0 | 18        |
| 6  | Molecular modeling of MCPA herbicide adsorption by goethite (110) surface in dependence of pH. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.   | 0.5 | 3         |
| 7  | Energy transfer mechanism in luminescence Eu(III) and Tb(III) complexes of coumarin-3-carboxylic acid: A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 240, 118591.  | 2.0 | 12        |
| 8  | Synthesis, X-ray structure, and DFT modeling of a new polymeric zinc(II) complex of 2-mercaptonicotinic acid (MntH), {[Zn(Mnt <sup>-</sup> Mnt)(en)] <sub>n</sub> ·nH <sub>2</sub> O}. <i>Monatshefte für Chemie</i> , 2019, 150, 219-231.   | 0.9 | 3         |
| 9  | Periodic DFT modeling and vibrational analysis of silver(I) cyanide complexes of thioureas. <i>Journal of Molecular Modeling</i> , 2019, 25, 90.   | 0.8 | 8         |
| 10 | X-ray structures, solid state periodic DFT modeling and vibrational study of alkylenediammonium hexachlorostannates compounds NH <sub>3</sub> (CH <sub>2</sub> ) <sub>n</sub> NH <sub>3</sub> SnCl <sub>6</sub> (n = 3, 4, 5). <i>Journal of Molecular Structure</i> , 2019, 1177, 55-67.  | 1.8 | 5         |
| 11 | Synthesis, characterization, DFT calculations and antimicrobial studies of cadmium(II) sulfate complexes of thioureas and 2-mercaptopyridine; X-ray structures of polymeric diaqua(N,N <sup>+</sup> -dimethylthiourea) sulfatocadmium(II) and bis(2-mercaptopyridine)sulfatocadmium(II). <i>Polyhedron</i> , 2018, 149, 126-133. | 1.0 | 3         |
| 12 | Synthesis, crystal structure and DFT studies of a novel dinuclear copper(I) complex with triphenylphosphine and 2-mercaptonicotinic acid. <i>Journal of Molecular Structure</i> , 2018, 1153, 179-186.   | 1.8 | 3         |
| 13 | Theoretical insight in highly luminescent properties of Eu(III) complex with phenanthroline. <i>Journal of Luminescence</i> , 2018, 202, 192-205.  | 1.5 | 28        |
| 14 | DFT study of the molecular and crystal structure and vibrational analysis of cisplatin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 176, 58-66.   | 2.0 | 28        |
| 15 | High-level <i>Ab Initio</i> Absorption Spectra Simulations of Neutral, Anionic and Neutral+ Chromophore of Green Fluorescence Protein Chromophore Models in Gas Phase and Solution. <i>Photochemistry and Photobiology</i> , 2017, 93, 1356-1367.  | 1.3 | 4         |
| 16 | Solid state DFT modeling and vibrational characterisation of butylenediammonium and hexylenediammonium hexafluorosilicate, NH <sub>3</sub> (CH <sub>2</sub> ) <sub>n</sub> NH <sub>3</sub> SiF <sub>6</sub> (n=4 and 6). <i>Vibrational Spectroscopy</i> , 2017, 88, 83-93.  | 1.2 | 11        |
| 17 | Synthesis, X-ray structure, spectroscopic (IR, NMR) analysis and DFT modeling of a new polymeric Zinc(II) complex of cystamine, [Zn(Cym-Cym)Cl <sub>2</sub> ]. <i>Polyhedron</i> , 2017, 122, 105-115.   | 1.0 | 5         |
| 18 | Synthesis, spectroscopic characterization, DFT calculations and antimicrobial properties of silver(I) complexes of 2,2'-bipyridine and 1,10-phenanthroline. <i>Polyhedron</i> , 2016, 115, 212-218.  | 1.0 | 25        |

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|----|--|-----|-----------|
| 19 | Novel silver(I) complexes of coumarin oxyacetate ligands and their phenanthroline adducts: Biological activity, structural and spectroscopic characterisation. <i>Journal of Inorganic Biochemistry</i> , 2016, 163, 53-67.  | 1.5 | 23        |
| 20 | Intramolecular Charge-Transfer Excited-State Processes in 4-( <i>N,N</i> -Dimethylamino)benzonitrile: The Role of Twisting and the $\pi^*$ State. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6232-6243.   | 1.1 | 60        |
| 21 | Spectroscopic studies, DFT calculations, and cytotoxic activity of novel silver(I) complexes of hydroxy ortho-substituted-nitro-2H-chromen-2-one ligands and a phenanthroline adduct. <i>Journal of Inorganic Biochemistry</i> , 2015, 153, 103-113.                             | 1.5 | 18        |
| 22 | Adsorption of the Herbicide 4-Chloro-2-methylphenoxyacetic Acid (MCPA) by Goethite. <i>Environmental Science &amp; Technology</i> , 2014, 48, 11803-11810.   | 4.6 | 38        |
| 23 | Lanthanide and transition metal complexes of bioactive coumarins: Molecular modeling and spectroscopic studies. <i>Journal of Inorganic Biochemistry</i> , 2014, 135, 100-112.   | 1.5 | 28        |
| 24 | Effect of the metal-metal interactions on the absorption properties of Pt(II) and Pd(II) complexes of glyoxilic acid oxime in solution and solid state: Theoretical and experimental study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 267, 35-48.   | 2.0 | 6         |
| 25 | NMR, IR and DFT studies of phenylplatinum complexes with O-monodentate coordinated silsesquioxanate and auxiliary phosphine ligands. <i>Journal of Organometallic Chemistry</i> , 2012, 697, 23-32.  | 0.8 | 2         |
| 26 | DFT modeling, UV-Vis and IR spectroscopic study of acetylacetone-modified zirconia sol-gel materials. <i>Journal of Molecular Modeling</i> , 2012, 18, 2409-2422.  | 0.8 | 58        |
| 27 | First principles study of structure and properties of La- and Mn-modified BiFeO <sub>3</sub> . <i>Solid State Sciences</i> , 2012, 14, 782-788.  | 1.5 | 19        |
| 28 | Molecular structure and spectroscopic studies on novel complexes of coumarin-3-carboxylic acid with Ni(II), Co(II), Zn(II) and Mn(II) ions based on density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 84, 275-285. | 2.0 | 26        |
| 29 | Synthesis and characterization of a dinuclear platinum complex with silsesquioxanate ligand. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 1738-1743.  | 0.8 | 7         |
| 30 | DFT, IR, Raman and NMR study of the coordination ability of coumarin-3-carboxylic acid to Pr(III). <i>Journal of Molecular Structure</i> , 2010, 979, 115-121.   | 1.8 | 14        |
| 31 | Coordination properties of warfarin towards Pr(III) predicted from DFT and FT-IR studies. <i>Chemical Physics</i> , 2010, 374, 37-45.  | 0.9 | 5         |
| 32 | Solvatochromic and Ionochromic Effects of Iron(II)bis(1,10-phenanthroline)dicyano: a Theoretical Study. <i>Inorganic Chemistry</i> , 2010, 49, 1634-1646.  | 1.9 | 26        |
| 33 | Is the CO frequency shift a reliable indicator of coumarin binding to metal ions through the carbonyl oxygen?. <i>Chemical Physics</i> , 2009, 365, 69-79.   | 0.9 | 17        |
| 34 | Multiple adsorption of NO on cobalt-exchanged chabazite, mordenite, and ferrierite zeolites: A periodic density functional theory study. <i>Journal of Chemical Physics</i> , 2009, 131, 054101.   | 1.2 | 8         |
| 35 | DFT-based molecular modeling and vibrational study of the La(III) complex of 3,3'-bis(benzylidene)bis(4-hydroxycoumarin). <i>Journal of Molecular Modeling</i> , 2008, 14, 353-366.  | 0.8 | 33        |
| 36 | Experimental and Theoretical Studies on Biologically Active Lanthanide (III) Complexes. , 2008, , .  |     | 1         |

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|----|--|-----|-----------|
| 37 | Spectroscopic and Theoretical Studies of a New Cerium (III) Complex with 3,3'-bis(ortho-pyridinomethylene)di[4-hydroxycoumarin]. <i>Spectroscopy Letters</i> , 2007, 40, 65-81.  | 0.5 | 10        |
| 38 | Bonding Analyses, Formation Energies, and Vibrational Properties of $M^{R<sub>2</sub>}$ Complexes (M = Ag(I), Ni(II), Cu(II), or Zn(II)). <i>Journal of Physical Chemistry A</i> , 2007, 111, 13075-13087.   | 1.1 | 31        |
| 39 | Excited-State Proton Transfer in 7-Hydroxy-4-methylcoumarin along a Hydrogen-Bonded Water Wire. <i>Journal of Physical Chemistry A</i> , 2007, 111, 127-135.   | 1.1 | 43        |
| 40 | Theoretical Study of Metal-Ligand Interaction in Sm(III), Eu(III), and Tb(III) Complexes of Coumarin-3-Carboxylic Acid in the Gas Phase and Solution. <i>Inorganic Chemistry</i> , 2007, 46, 10926-10936.  | 1.9 | 27        |
| 41 | Vibrational and theoretical study of coumarin-3-carboxylic acid binding mode in Ce(III) and Nd(III) complexes. <i>Vibrational Spectroscopy</i> , 2007, 44, 78-88.  | 1.2 | 21        |
| 42 | Theoretical study of the substituent effect on the intramolecular hydrogen bonds in di(4-hydroxycoumarin) derivatives. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1304-1315.   | 1.0 | 12        |
| 43 | Spectroscopic and theoretical study of Cu(II), Zn(II), Ni(II), Co(II) and Cd(II) complexes of glyoxilic acid oxime. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 63, 403-415.  | 2.0 | 44        |
| 44 | Comprehensive DFT and MO studies on glyoxilic acid oxime and related ions in gas phase and solution: Conformations, basicities and acidities. <i>Chemical Physics</i> , 2006, 321, 311-324.  | 0.9 | 12        |
| 45 | DFT modeling and spectroscopic study of metal-ligand bonding in La(III) complex of coumarin-3-carboxylic acid. <i>Chemical Physics</i> , 2006, 327, 209-219.   | 0.9 | 52        |
| 46 | Raman, FT-IR and DFT studies of ortho-, meta- and para-pyridinomethylene substituted di(4-hydroxy-coumarin) and their Ce(III), La(III) and Nd(III) complexes. <i>Journal of Raman Spectroscopy</i> , 2006, 37, 742-754.  | 1.2 | 15        |
| 47 | Characteristic Raman and IR bands of 3,3'-benzylidenebis(4-hydroxycoumarin) and its La(III), Ce(III) and Nd(III) complexes. <i>Journal of Raman Spectroscopy</i> , 2006, 37, 808-815.  | 1.2 | 10        |
| 48 | Coordination Properties of the Oxime Analogue of Glycine to Cu(II). <i>Journal of Physical Chemistry A</i> , 2005, 109, 5668-5676.   | 1.1 | 46        |
| 49 | Excited State Properties of 7-Hydroxy-4-methylcoumarin in the Gas Phase and in Solution. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11860-11869.   | 1.1 | 62        |
| 50 | Synthesis and Spectroscopic Study of a New Lanthanum(III) Complex of 3,3'-Benzylidenedi[4-hydroxycoumarin]. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2004, 34, 1635-1650.   | 1.8 | 7         |
| 51 | Effect of the nature of mendixan $\pi$ - $\pi$ X $\pi$ interactions (X= Na $\pi$ , Cu $\pi$ , H $\pi$ ) and the hydrogen bonding on the $\frac{1}{2}(C\pi \dots O)$ behavior: theoretical and spectroscopic study. <i>Chemical Physics</i> , 2004, 300, 119-131.   | 0.9 | 13        |
| 52 | Vibrational properties of glyoxilic acid oxime dimers and tetramer. <i>Vibrational Spectroscopy</i> , 2003, 31, 143-154.   | 1.2 | 2         |
| 53 | Vibrational study of new Pt(II) and Pd(II) complexes with functionalized nitrogen-containing tertiary phosphine oxides. Ab initio study of ortho-, meta- and para-dimethylphosphinylmethyleneoxyaniline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2003, 59, 169-192. | 2.0 | 6         |
| 54 | DFT study of hydrogen-bonded dimers and tetramer of glyoxilic acid oxime. <i>Chemical Physics</i> , 2003, 286, 205-217.  | 0.9 | 12        |

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|----|--|-----|-----------|
| 55 | Conformational stability and vibrational spectrum of glyoxilic acid oxime predicted from ab initio study. <i>Journal of Molecular Structure</i> , 2002, 604, 211-220.  | 1.8 | 9         |
| 56 | IR study of the N,N <sup>2</sup> ,N <sup>3</sup> -triphenylguanidine and its imine nitrogen coordinated Pd(II) complexes. <i>Vibrational Spectroscopy</i> , 2001, 27, 153-164.   | 1.2 | 14        |
| 57 | Barriers to Internal Rotation and Conformational Behaviour of the MESO and D,L Isomers of Pt(II) Complexes with Antitumour Activity. <i>Journal of Coordination Chemistry</i> , 2000, 51, 305-317.   | 0.8 | 0         |
| 58 | Synthesis and vibrational study of platinum(II) and palladium(II) complexes of glyoxilic acid oxime. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1999, 55, 2849-2859.   | 2.0 | 9         |
| 59 | Ab initio study of 1,1-(methylphosphinylidene) bis(methanamine) and vibrational assignment of its N,N <sup>2</sup> -coordinated Pt(II) and Pd(II) chloro complexes. <i>Vibrational Spectroscopy</i> , 1999, 20, 133-142.   | 1.2 | 3         |
| 60 | Novel platinum (II) complexes with (pyridyloxymethylene)dimethylphosphine oxides-synthesis, IR and Raman study.. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1998, 54, 477-490.   | 2.0 | 4         |
| 61 | Platinum (II) Compounds With Antitumor Activity Studied by Molecular Mechanics. <i>Metal-Based Drugs</i> , 1998, 5, 91-102.  | 3.8 | 2         |
| 62 | Molecular mechanical and quantum chemical study of the species involved in the hydrolysis of cis-diamminedichloroplatinum(II) and substituted bis(ethylenediamine)-dichloroplatinum(II) complexes II. Simulated transition states. <i>Monatshefte für Chemie</i> , 1997, 128, 443-474. | 0.9 | 5         |
| 63 | Molecular mechanics modelling of Pt(II) complexes with antitumor activity. Influence of the type and the positions of the ring substituents on the conformational energies and thermodynamic stabilities. <i>Monatshefte für Chemie</i> , 1997, 128, 1119-1132.                        | 0.9 | 2         |
| 64 | IR and Raman study of Pt(II) and Pd(II) complexes of amino substituted phosphine oxides. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 819-828.   | 2.0 | 12        |