T M Dudev

List of Publications by Year
in descending order

112 papers	4,415 citations	126708 33 h-index	114278 63 g-index
116 all docs	116 docs citations	116 times ranked	4955 citing authors

#	Article	IF	Citations
1	A DFT/PCM Study on the Affinity of Salinomycin to Bind Monovalent Metal Cations. Molecules, 2022, 27, 532.	1.7	3
2	Complexation of trivalent metal cations (Al³⁺, Ga³⁺, In³⁺,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 governing the hostâ€“guest recognition. Physical Chemistry Chemical Physics, 2022, 24, 6274-6281.	1.3	4
3	Theoretical Insight into the Phosphate-Targeted Silverâ€™s Antibacterial Action: Differentiation between Gram (+) and Gram (â^') Bacteria. Inorganic Chemistry, 2022, 61, 10089-10100.	1.9	6
4	Competition between abiogenic and biogenic metal cations in biological systems: Mechanisms of galliumâ€˜s anticancer and antibacterial effect. Journal of Inorganic Biochemistry, 2021, 214, 111309.	1.5	21
5	Hostâ€“Guest Complexation of Cucurbit[7]Uril and Cucurbit[8]Uril with the Antineoplastic and Multiple Sclerosis Agent Mitoxantrone (Novantrone). Journal of Physical Chemistry A, 2021, 125, 536-542.	1.1	6
6	Metal Affinity/Selectivity of Monophosphate-Containing Signaling/Lipid Molecules. Journal of Chemical Theory and Computation, 2021, 17, 2444-2456.	2.3	6
7	Trinuclear Calcium Site in the C2 Domain of PKCÎ±/Î³ Is Prone to Lithium Attack. ACS Omega, 2021, 6, 20657-20666.	1.6	5
8	Strontium Binding to Î±-Parvalbumin, a Canonical Calcium-Binding Protein of the â€œEF-Handâ€•Family. Biomolecules, 2021, 11, 1158.	1.8	11
9	Calcium in Signaling: Its Specificity and Vulnerabilities toward Biogenic and Abiogenic Metal Ions. Journal of Physical Chemistry B, 2021, 125, 10419-10431.	1.2	6
10	Ca2+/Sr2+ Selectivity in Calcium-Sensing Receptor (CaSR): Implications for Strontiumâ€™s Anti-Osteoporosis Effect. Biomolecules, 2021, 11, 1576.	1.8	19
11	How mechanical forces can modulate the metal affinity and selectivity of metal binding sites in proteins. Metallomics, 2020, 12, 363-370.	1.0	4
12	Inclusion complexes of ibuprofen and Î²-cyclodextrin: Supramolecular structure and stability. Journal of Molecular Structure, 2020, 1205, 127575.	1.8	21
13	Zinc and Its Critical Role in Retinitis pigmentosa: Insights from DFT/SMD Calculations. Inorganic Chemistry, 2020, 59, 17347-17355.	1.9	10
14	Synthesis, Photophysical Characterization, and Sensor Activity of New 1,8-Naphthalimide Derivatives. Sensors, 2020, 20, 3892.	2.1	6
15	Complexation of biologically essential (mono- and divalent) metal cations to cucurbiturils: a DFT/SMD evaluation of the key factors governing the hostâ€“guest recognition. RSC Advances, 2020, 10, 28139-28147.	1.7	10
16	Factors governing the competition between group IA and IB cations for monensin A: a DFT/PCM study. RSC Advances, 2020, 10, 5734-5741.	1.7	2
17	Gallium as an Antibacterial Agent: A DFT/SMD Study of the Ga³⁺/Fe³⁺ Competition for Binding Bacterial Siderophores. Inorganic Chemistry, 2020, 59, 6242-6254.	1.9	36
18	Water inside Î²-cyclodextrin cavity: amount, stability and mechanism of binding. Beilstein Journal of Organic Chemistry, 2019, 15, 1592-1600.	1.3	43

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19	Electric field influence on the helical structure of peptides: insights from DFT/PCM computations. Physical Chemistry Chemical Physics, 2019, 21, 16198-16206.	1.3	8
20	Hostâ€“guest interactions between p-sulfonatocalix[4]arene and p-sulfonatothiacalix[4]arene and group IA, IIA and f-block metal cations: a DFT/SMD study. Beilstein Journal of Organic Chemistry, 2019, 15, 1321-1330.	1.3	8
21	Free and Bound Therapeutic Lithium in Brain Signaling. Accounts of Chemical Research, 2019, 52, 2960-2970.	7.6	12
22	Novel Insights into Galliumâ€™s Mechanism of Therapeutic Action: A DFT/PCM Study of the Interaction between Ga³⁺ and Ribonucleotide Reductase Substrates. Journal of Physical Chemistry B, 2019, 123, 5444-5451.	1.2	13
23	Why Cellular Di/Triphosphates Preferably Bind Mg²⁺ and Not Ca²⁺. Journal of Chemical Theory and Computation, 2019, 15, 6992-7003.	2.3	10
24	Hydroxamic acid derivatives as histone deacetylase inhibitors: a DFT study of their tautomerism and metal affinities/selectivities. Journal of Molecular Modeling, 2018, 24, 114.	0.8	6
25	Competition between abiogenic Al3+ and native Mg2+, Fe2+ and Zn2+ ions in protein binding sites: implications for aluminum toxicity. Journal of Molecular Modeling, 2018, 24, 55.	0.8	20
26	Competition between Li⁺and Na⁺in sodium transporters and receptors: Which Na⁺-Binding sites are â€œtherapeuticâ€•Li⁺targets?. Chemical Science, 2018, 9, 4093-4103.	3.7	22
27	How Pb²⁺ Binds and Modulates Properties of Ca²⁺-Signaling Proteins. Inorganic Chemistry, 2018, 57, 14798-14809.	1.9	35
28	How an electric field can modulate the metal ion selectivity of protein binding sites: insights from DFT/PCM calculations. Physical Chemistry Chemical Physics, 2018, 20, 24633-24640.	1.3	19
29	How Native and Non-Native Cations Bind and Modulate the Properties of GTP/ATP. Journal of Chemical Theory and Computation, 2018, 14, 3311-3320.	2.3	9
30	How First Shellâ€“Second Shell Interactions and Metal Substitution Modulate Protein Function. Inorganic Chemistry, 2018, 57, 14052-14061.	1.9	5
31	Factors Governing the Hostâ€“Guest Interactions between IIA/IIB Group Metal Cations and Î±-Cyclodextrin: A DFT/CDM Study. Inorganic Chemistry, 2017, 56, 1981-1987.	1.9	20
32	How the extra methylene group affects the ligation properties of Glu vs. Asp and Gln vs. Asn amino acids: a DFT/PCM study. Journal of Molecular Modeling, 2017, 23, 45.	0.8	5
33	Determinants of the hostâ€“guest interactions between Î±-, Î²- and Î³-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study. Physical Chemistry Chemical Physics, 2017, 19, 15129-15136.	1.3	15
34	Î±-Cyclodextrin: How Effectively Can Its Hydrophobic Cavity Be Hydrated?. Journal of Physical Chemistry B, 2017, 121, 9260-9267.	1.2	20
35	How Native and Alien Metal Cations Bind ATP: Implications for Lithium as a Therapeutic Agent. Scientific Reports, 2017, 7, 42377.	1.6	42
36	Determinants of Fe²⁺ over M²⁺ (M = Mg, Mn, Zn) Selectivity in Non-Heme Iron Proteins. Inorganic Chemistry, 2016, 55, 12644-12650.	1.9	15

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37	Preferred Hydrogen-Bonding Partners of Cysteine: Implications for Regulating Cys Functions. Journal of Physical Chemistry B, 2016, 120, 10288-10296.	1.2	57
38	Influence of the Selectivity Filter Properties on Proton Selectivity in the Influenza A M2 Channel. Journal of the American Chemical Society, 2016, 138, 13038-13047.	6.6	6
39	Factors controlling the selectivity for Na⁺over Mg²⁺in sodium transporters and enzymes. Physical Chemistry Chemical Physics, 2016, 18, 16986-16997.	1.3	17
40	Gallium as a Therapeutic Agent: A Thermodynamic Evaluation of the Competition between Ga³⁺ and Fe³⁺ Ions in Metalloproteins. Journal of Physical Chemistry B, 2016, 120, 2241-2248.	1.2	44
41	Potassium Versus Sodium Selectivity in Monovalent Ion Channel Selectivity Filters. Metal Ions in Life Sciences, 2016, 16, 325-347.	2.8	6
42	Ion Selectivity in the Selectivity Filters of Acid-Sensing Ion Channels. Scientific Reports, 2015, 5, 7864.	1.6	19
43	Cyclodextrin-Based Solidâ€“Gas Clathrates. Journal of Agricultural and Food Chemistry, 2015, 63, 6603-6613.	2.4	14
44	Selectivity Mechanism of the Voltage-gated Proton Channel, HV1. Scientific Reports, 2015, 5, 10320.	1.6	53
45	Quantumâ€chemistry based calibration of the alkali metal cation series (Li⁺ï£¿Cs⁺) for largeâ€scale polarizable molecular mechanics/dynamics simulations. Journal of Computational Chemistry, 2015, 36, 285-302.	1.5	12
46	Competition among Metal Ions for Protein Binding Sites: Determinants of Metal Ion Selectivity in Proteins. Chemical Reviews, 2014, 114, 538-556.	23.0	329
47	Wnt and lithium: a common destiny in the therapy of nervous system pathologies?. Cellular and Molecular Life Sciences, 2014, 71, 1123-1148.	2.4	52
48	Ion Selectivity Strategies of Sodium Channel Selectivity Filters. Accounts of Chemical Research, 2014, 47, 3580-3587.	7.6	64
49	Modeling Zn²⁺ Release From Metallothionein. Journal of Physical Chemistry A, 2014, 118, 9244-9252.	1.1	12
50	Evolution of Eukaryotic Ion Channels: Principles Underlying the Conversion of Ca²⁺-Selective to Na⁺-Selective Channels. Journal of the American Chemical Society, 2014, 136, 3553-3559.	6.6	20
51	Differential Role of the Protein Matrix on the Binding of a Catalytic Aspartate to Mg²⁺ vs Ca²⁺: Application to Ribonuclease H. Journal of the American Chemical Society, 2013, 135, 6541-6548.	6.6	20
52	Importance of Metal Hydration on the Selectivity of Mg²⁺ versus Ca²⁺ in Magnesium Ion Channels. Journal of the American Chemical Society, 2013, 135, 17200-17208.	6.6	53
53	Calcium Ion Selectivity in Biological Systems. , 2013, , 478-484.		5
54	Why voltage-gated Ca2+ and bacterial Na+ channels with the same EEEE motif in their selectivity filters confer opposite metal selectivity. Physical Chemistry Chemical Physics, 2012, 14, 12451.	1.3	34

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55	Competition among Ca²⁺, Mg²⁺, and Na⁺ for Model Ion Channel Selectivity Filters: Determinants of Ion Selectivity. Journal of Physical Chemistry B, 2012, 116, 10703-10714.	1.2	45
56	The effect of metal binding on the characteristic infrared band intensities of ligands of biological interest. Journal of Molecular Structure, 2012, 1009, 83-88.	1.8	12
57	Competition between Li⁺ and Mg²⁺ in Metalloproteins. Implications for Lithium Therapy. Journal of the American Chemical Society, 2011, 133, 9506-9515.	6.6	74
58	Factors Governing the Na⁺ vs K⁺ Selectivity in Sodium Ion Channels. Journal of the American Chemical Society, 2010, 132, 2321-2332.	6.6	83
59	Factors Controlling the Mechanism of NAD+Non-Redox Reactions. Journal of the American Chemical Society, 2010, 132, 16533-16543.	6.6	14
60	Metal-Binding Affinity and Selectivity of Nonstandard Natural Amino Acid Residues from DFT/CDM Calculations. Journal of Physical Chemistry B, 2009, 113, 11754-11764.	1.2	23
61	Determinants of K⁺ vs Na⁺ Selectivity in Potassium Channels. Journal of the American Chemical Society, 2009, 131, 8092-8101.	6.6	90
62	Metal Binding Affinity and Selectivity in Metalloproteins: Insights from Computational Studies. Annual Review of Biophysics, 2008, 37, 97-116.	4.5	205
63	Mononuclear versus Binuclear Metal-Binding Sites:â€‰ Metal-Binding Affinity and Selectivity from PDB Survey and DFT/CDM Calculations. Journal of the American Chemical Society, 2008, 130, 3844-3852.	6.6	35
64	Effect of Carboxylate-Binding Mode on Metal Binding/Selectivity and Function in Proteins. Accounts of Chemical Research, 2007, 40, 85-93.	7.6	109
65	All-Electron Calculations of the Nucleation Structures in Metal-Induced Zinc-Finger Folding:â€‰ Role of the Peptide Backbone. Journal of the American Chemical Society, 2007, 129, 12497-12504.	6.6	20
66	Competition between Protein Ligands and Cytoplasmic Inorganic Anions for the Metal Cation:Â A DFT/CDM Study. Journal of the American Chemical Society, 2006, 128, 10541-10548.	6.6	13
67	A DFT/CDM Study of Metalâ"Carboxylate Interactions in Metalloproteins:Â Factors Governing the Maximum Number of Metal-Bound Carboxylates. Journal of the American Chemical Society, 2006, 128, 1553-1561.	6.6	55
68	Factors Governing the Metal Coordination Number in Metal Complexes from Cambridge Structural Database Analyses. Journal of Physical Chemistry B, 2006, 110, 1889-1895.	1.2	117
69	Factors Governing the Substitution of La3+for Ca2+and Mg2+in Metalloproteins:Â A DFT/CDM Study. Journal of the American Chemical Society, 2005, 127, 4091-4103.	6.6	56
70	Monodentate versus Bidentate Carboxylate Binding in Magnesium and Calcium Proteins:Â What Are the Basic Principles?. Journal of Physical Chemistry B, 2004, 108, 4546-4557.	1.2	114
71	Oxyanion Selectivity in Sulfate and Molybdate Transport Proteins:Â An ab Initio/CDM Study. Journal of the American Chemical Society, 2004, 126, 10296-10305.	6.6	23
72	Principles Governing Mg, Ca, and Zn Binding and Selectivity in Proteins. ChemInform, 2003, 34, no.	0.1	0

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73	Principles Governing Mg, Ca, and Zn Binding and Selectivity in Proteins. Chemical Reviews, 2003, 103, 773-788.	23.0	421
74	A Combined Experimental and Theoretical Study of Divalent Metal Ion Selectivity and Function in Proteins:Â Application toE. coliRibonuclease H1. Journal of the American Chemical Society, 2003, 125, 9318-9328.	6.6	61
75	Firstâ^'Second Shell Interactions in Metal Binding Sites in Proteins:Â A PDB Survey and DFT/CDM Calculations. Journal of the American Chemical Society, 2003, 125, 3168-3180.	6.6	189
76	Metal Binding and Selectivity in Zinc Proteins. Journal of the Chinese Chemical Society, 2003, 50, 1093-1102.	0.8	33
77	Factors Governing the Protonation State of Cysteines in Proteins:Â An Ab Initio/CDM Study. Journal of the American Chemical Society, 2002, 124, 6759-6766.	6.6	100
78	Metal Selectivity in Metalloproteins:Â Zn2+vs Mg2+. Journal of Physical Chemistry B, 2001, 105, 4446-4452.	1.2	68
79	Modeling Zn2+â^'Cysteinate Complexes in Proteins. Journal of Physical Chemistry B, 2001, 105, 10709-10714.	1.2	43
80	Effective bond charges from infrared intensities in CH4, SiH4, GeH4 and SnH4. Journal of Molecular Structure, 2001, 565-566, 395-398.	1.8	3
81	Raman spectroscopy of carbon-containing particles. Vibrational Spectroscopy, 2001, 26, 179-186.	1.2	220
82	Tetrahedral vs Octahedral Zinc Complexes with Ligands of Biological Interest:â€‰ A DFT/CDM Study. Journal of the American Chemical Society, 2000, 122, 11146-11153.	6.6	201
83	Metal Binding in Proteins:Â The Effect of the Dielectric Medium. Journal of Physical Chemistry B, 2000, 104, 3692-3694.	1.2	54
84	Design, Synthesis, and SAR of Novel Carbapenem Antibiotics with High Stability to Xanthomonas maltophilia Oxyiminocephalosporinase Type II. Journal of Medicinal Chemistry, 2000, 43, 3632-3640.	2.9	18
85	Competitive Binding in Magnesium Coordination Chemistry:â€‰ Water versus Ligands of Biological Interest. Journal of the American Chemical Society, 1999, 121, 7665-7673.	6.6	149
86	Incremental Binding Free Energies in Mg2+ Complexes:â€‰ A DFT Study. Journal of Physical Chemistry A, 1999, 103, 8093-8100.	1.1	45
87	Creation of intensity theory in vibrational spectroscopy: Key role of ab initio quantum mechanical calculations. International Journal of Quantum Chemistry, 1998, 70, 331-339.	1.0	4
88	Ring Strain Energies from ab Initio Calculations. Journal of the American Chemical Society, 1998, 120, 4450-4458.	6.6	227
89	Ab initio calculations of Raman intensity parameters and geometry of polyynes and polyynenitriles. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 2053-2059.	2.0	5
90	1H and 13C NMR study and AM1 calculations of some azobenzenes and N-benzylideneanilines: effect of substituents on the molecular planarity. Journal of Molecular Structure, 1997, 412, 153-159.	1.8	22

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91	Interpretation of carbonyl stretching band intensities in the infrared spectra: an ab initio MO study. Journal of Molecular Structure, 1997, 406, 119-125.	1.8	15
92	Effective bond charges from infrared and Raman intensities. Journal of Molecular Structure, 1997, 408-409, 57-62.	1.8	1
93	Nâ€“H stretching frequencies and the conformation of substituted ureas: an ab initio MO study. Journal of Molecular Structure, 1997, 407, 47-51.	1.8	12
94	Molecular geometry, vibrational frequencies, infrared intensities and Cî—¼N effective bond charges in a series of simple nitrile compounds: HF/6â€“31+G(d,p) molecular orbital study. Journal of Molecular Structure, 1997, 436-437, 427-433.	1.8	9
95	Predicted Raman Intensities of CH3CCH, CH3CCD, CD3CCH, CD3CCD and12CH313C13CH. Journal of Raman Spectroscopy, 1997, 28, 199-204.	1.2	0
96	Interpretation of Raman intensities: effective induced bond charges from atomic polarizability tensors. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1996, 52, 527-538.	2.0	3
97	Effective bond charges from infrared intensities: ab initio calculations. Journal of Molecular Structure, 1996, 377, 75-79.	1.8	6
98	Effective bond charges from experimental IR intensities. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1995, 51, 739-754.	2.0	13
99	Rotational contributions to polarizability derivatives from Raman spectra. Journal of Raman Spectroscopy, 1993, 24, 113-117.	1.2	4
100	Relationship between atomic polarizability tensors and valence optical theories of Raman intensities. Journal of Raman Spectroscopy, 1993, 24, 877-882.	1.2	3
101	Interpretation of vibrational absorption intensities: Effective bond charges from rotation free atomic polar tensors. Spectrochimica Acta Part A: Molecular Spectroscopy, 1993, 49, 373-385.	0.1	12
102	Raman and infrared study of amorphous SeTe/CdSe superlattices. Applied Physics A: Solids and Surfaces, 1992, 55, 203-206.	1.4	6
103	Relationship between infrared intensity theories: Electro-optical parameters and bond polar parameters. Spectrochimica Acta Part A: Molecular Spectroscopy, 1992, 48, 1153-1163.	0.1	4
104	Vibrational intensity analysis of 1,2-dichloroethane and 1-chloropropane. Vibrational Spectroscopy, 1992, 3, 9-21.	1.2	6
105	Infrared spectra of Langmuirâ€”Blodgett multilayers of docosylammonium phosphate. Colloids and Surfaces, 1991, 60, 351-368.	0.9	17
106	Relationship Between Infrared Intensity Theories: Electro-Optical Parameters And Bond Polar Parameters. Proceedings of SPIE, 1989, , .	0.8	0
107	Computations in vibrational intensity spectroscopy. Journal of Molecular Structure, 1988, 173, 111-128.	1.8	9
108	Interpretation of infrared intensities of some simple hydrides. Journal of Molecular Structure, 1987, 157, 289-294.	1.8	5

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109	Predicted infrared intensities of diacetylene and 1,3-pentadiyne. Journal of Molecular Spectroscopy, 1986, 120, 276-283.	0.4	4
110	Interpretation and prediction of vibrational intensities in infrared spectra: fluorinated methanes. Journal of Molecular Structure, 1986, 145, 1-13.	1.8	9
111	Infrared intensities. an mo study of the transferability of bond polar parameters. Journal of Molecular Structure, 1985, 129, 27-33.	1.8	3
112	Factors governing the affinity and selectivity of histone deacetylase inhibitors for the HDAC8 enzyme active site: Implications for anticancer therapy. Journal of Physical Organic Chemistry, 0, , e4268.	0.9	0