Reza Behjatmanesh-Ardakani

List of Publications by Year
in descending order

62 papers	1,138 citations	361413 20 h-index	434195 31 g-index
63 all docs	63 docs citations	63 times ranked	544 citing authors

#	Article	IF	Citations
1	New oxovanadium and dioxomolybdenum complexes as catalysts for sulfoxidation: experimental and theoretical investigations of E and Z isomers of ONO tridentate Schiff base ligand. Journal of Sulfur Chemistry, 2022, 43, 22-36.	2.0	22
2	Diverse coordination of isoniazid hydrazone Schiff base ligand towards iron(III): Synthesis, characterization, SC-XRD, HSA, QTAIM, MEP, NCI, NBO and DFT study. Journal of Molecular Structure, 2022, 1250, 131691.	3.6	44
3	A mechanistic periodic DFT study on the dissociation of tetrachlorodibenzofuran (TCDF) by M-doped carbon nanotube catalysts (MÂ=ÂAl, Fe, Mn). Applied Surface Science, 2022, 579, 152217.	6.1	3
4	Magnetic Nanoparticle-Supported Basic Ionic Liquid: A Reusable Phase-Transfer Catalyst for Knoevenagel Condensation in Aqueous Medium. Russian Journal of Organic Chemistry, 2022, 58, 144-151.	0.8	0
5	Synthesis, spectral characterization, and theoretical investigation of Ni(II) and Pd(II) complexes incorporating symmetrical tetradentate Schiff base ligand: Suzuki-Miyaura cross-coupling reaction using PdLSym. Journal of the Iranian Chemical Society, 2022, 19, 3981-3992.	2.2	9
6	Synthesis, crystal structure, spectral characterization, catalytic studies and computational studies of Ni(II) and Pd(II) complexes of symmetrical tetradentate Schiff base ligand. Journal of Coordination Chemistry, 2022, 75, 972-993.	2.2	18
7	Novel copper(II) and zinc(II) complexes of halogenated bidentate N,O-donor Schiff base ligands: Synthesis, characterization, crystal structures, DNA binding, molecular docking, DFT and TD-DFT computational studies. Inorganica Chimica Acta, 2021, 514, 120004.	2.4	74
8	Synthesis, characterization, crystal structures, DFT, TD-DFT, molecular docking and DNA binding studies of novel copper(II) and zinc(II) complexes bearing halogenated bidentate N,O-donor Schiff base ligands. Polyhedron, 2021, 195, 114988.	2.2	76
9	Synthesis, crystal structure, theoretical calculation, spectroscopic and antibacterial activity studies of copper(II) complexes bearing bidentate schiff base ligands derived from 4-aminoantipyrine: Influence of substitutions on antibacterial activity. Journal of Molecular Structure, 2021, 1230, 129908.	3.6	87
10	Selective oxidation of benzyl alcohols to benzaldehydes catalyzed by dioxomolybdenum Schiff base complex: synthesis, spectral characterization, crystal structure, theoretical and computational studies. Transition Metal Chemistry, 2021, 46, 437.	1.4	33
11	Oxovanadium and dioxomolybdenum complexes: synthesis, crystal structure, spectroscopic characterization and applications as homogeneous catalysts in sulfoxidation. Journal of Coordination Chemistry, 2021, 74, 1563-1583.	2.2	27
12	Ultrasound-based synthesis, SC-XRD, NMR, DFT, HSA of new Schiff bases derived from 2-aminopyridine: Experimental and theoretical studies. Journal of Molecular Structure, 2021, 1233, 130105.	3.6	50
13	Band gap reduction of (Mo+N) co-doped TiO2 nanotube arrays with a significant enhancement in visible light photo-conversion: A combination of experimental and theoretical study. International Journal of Hydrogen Energy, 2021, 46, 21475-21498.	7.1	19
14	Synthesis, characterization, crystal structures, Hirshfeld surface analysis, DFT computational studies and catalytic activity of novel oxovanadium and dioxomolybdenum complexes with ONO tridentate Schiff base ligand. Polyhedron, 2021, 202, 115194.	2.2	62
15	A mechanistic periodic DFT study of CH, CO, and OH dissociations in methanol: M-doped carbon nanotubes (M=Pt, B, Al, N, P) versus Pt(100), Pt(110) and Pt(111) surfaces. Molecular Catalysis, 2021, 512, 111781.	2.0	2
16	Novel oxovanadium and dioxomolybdenum complexes of tridentate ONO-donor Schiff base ligand: Synthesis, characterization, crystal structures, Hirshfeld surface analysis, DFT computational studies and catalytic activity for the selective oxidation of benzylic alcohols. Inorganica Chimica Acta, 2021, 523, 120414.	2.4	56
17	Synthesis, crystal structure determination, Hirshfeld surface analysis, spectral characterization, theoretical and computational studies of titanium(IV) Schiff base complex. Journal of Coordination Chemistry, 2021, 74, 2682-2700.	2.2	19
18	Titanium(IV) complex containing ONO-tridentate Schiff base ligand: Synthesis, crystal structure determination, Hirshfeld surface analysis, spectral characterization, theoretical and computational studies. Journal of Molecular Structure, 2021, 1241, 130653.	3.6	47

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19	Experimental and theoretical studies of new dioxomolybdenum complex: Synthesis, characterization and application as an efficient homogeneous catalyst for the selective sulfoxidation. Inorganica Chimica Acta, 2021, 527, 120568.	2.4	28
20	Sonication-assisted synthesis of new Schiff bases derived from 3-ethoxysalicylaldehyde: Crystal structure determination, Hirshfeld surface analysis, theoretical calculations and spectroscopic studies. Journal of Molecular Structure, 2021, 1243, 130782.	3.6	32
21	Synthesis, spectra (FT-IR, NMR) investigations, DFT, FMO, MEP, NBO analysis and catalytic activity of MoO2(VI) complex with ONO tridentate hydrazone Schiff base ligand. Journal of Molecular Structure, 2021, 1245, 131259.	3.6	34
22	Zn(II) complexes containing O,N,N,O-donor Schiff base ligands: synthesis, crystal structures, spectral investigations, biological activities, theoretical calculations and substitution effect on structures. Journal of Coordination Chemistry, 2021, 74, 2720-2740.	2.2	27
23	A computational study on the effect of Ni impurity and O-vacancy on the adsorption and dissociation of water molecules on the surface of anatase (101). Journal of Physics and Chemistry of Solids, 2020, 136, 109176.	4.0	12
24	The association of Ï€â€“Ï€ stacking and hydrogen bonding interactions in substituted Rebek imide with 2,6-di(isobutyramido)pyridine rings: theoretical insight into X-Rebek imide||pyr complexes. Structural Chemistry, 2020, 31, 747-754.	2.0	0
25	Molecular and dissociative adsorption of tetrachlorodibenzodioxin on M-doped graphenes (Mâ€‰=â€‰B, Al,) Tj ETQq1 1 0.784314	1.8	3
26	Electronic structure and characterization of the spectra of trans/cis tautomers of urocanic acid isomers: A diagnostic tool. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 400, 112652.	3.9	0
27	Insights into the mechanism of inhibition of phospholipase A2 by resveratrol: An extensive molecular dynamics simulation and binding free energy calculation. Journal of Molecular Graphics and Modelling, 2020, 100, 107649.	2.4	10
28	Knoevenagel condensation versus Michael addition reaction in ionic-liquid-catalyzed synthesis of hexahydroquinoline: a SMDâ€“DFT study. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	2
29	The topology impact on hydrogen storage capacity of Sc-decorated ever-increasing porous graphene. Journal of Molecular Modeling, 2020, 26, 96.	1.8	3
30	Dispersion of Defects in TiO2 Semiconductor: Oxygen Vacancies in the Bulk and Surface of Rutile and Anatase. Catalysts, 2020, 10, 397.	3.5	44
31	Conformational switching of CO on graphene: the role of electric fields. Journal of Molecular Modeling, 2019, 25, 343.	1.8	1
32	Predictive Modeling of Corrosion in Al/Mg Dissimilar Joint. ChemEngineering, 2019, 3, 70.	2.4	2
33	A mechanistic study of photo-oxidation of phenol and AB92 by AgBr/TiO2. Research on Chemical Intermediates, 2019, 45, 4885-4896.	2.7	7
34	Synthesis, crystal structure, spectroscopic investigations, and computational studies of Ni(II) and Pd(II) complexes with asymmetric tetradentate NOON Schiff base ligand. Structural Chemistry, 2019, 30, 2289-2299.	2.0	33
35	Role of oxygen vacancy in the adsorption and dissociation of the water molecule on the surfaces of pure and Ni-doped rutile (110): a periodic full-potential DFT study. Surface Science, 2019, 679, 218-224.	1.9	31
36	Synthesis, crystal structure, experimental and theoretical studies of tetradentate N2O2 Schiff base ligand and its Ni(II) and Pd(II) complexes. Journal of the Iranian Chemical Society, 2019, 16, 1081-1090.	2.2	23

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37	Investigation of carboxylation of carbon nanotube in the adsorption of anti-cancer drug: A theoretical approach. Applied Surface Science, 2018, 427, 112-125.	6.1	21
38	Ammonia capture by MN₄ (Mâ€‰=â€‰Fe and Ni) clusters embedded in graphene. Journal of Coordination Chemistry, 2018, 71, 3476-3486.	2.2	9
39	Nickel(II) complex with an asymmetric tetradentate Schiff base ligand: synthesis, characterization, crystal structure, and DFT studies. Journal of Coordination Chemistry, 2018, 71, 3748-3762.	2.2	19
40	Full-potential DFT study of CO dissociation on Feâ€“Cu cluster. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	11
41	Periodic and non-periodic DFT modeling of CO reduction on the surface of Ni-doped graphene nanosheet. Molecular Catalysis, 2018, 455, 239-249.	2.0	8
42	Interaction between anti-cancer drug hydroxycarbamide and boron nitride nanotube: A long-range corrected DFT study. Computational and Theoretical Chemistry, 2017, 1117, 61-80.	2.5	19
43	Modelling phase equilibria of pure ionic liquids from a new equation of state. Ionics, 2016, 22, 2447-2459.	2.4	4
44	DFT-B3LYP study of interactions between host biphenyl-1-aza-18-crown-6 ether derivatives and guest Cd2+: NBO, NEDA, and QTAIM analyses. Journal of Molecular Modeling, 2016, 22, 149.	1.8	15
45	NBOâ€“NEDA, NPA, and QTAIM studies on the interactions between aza-, diaza-, and triaza-12-crown-4 (An-12-crown-4, n=1, 2, 3) and Li+, Na+, and K+ ions. Computational and Theoretical Chemistry, 2015, 1051, 62-71.	2.5	10
46	Modification of Tao-Mason equation of state: application to polymer melts. Physics and Chemistry of Liquids, 2014, 52, 17-25.	1.2	2
47	DFT-B3LYP and SMD study on the interactions between aza-, diaza-, and triaza-12-crown-4 (A n) Tj ETQq1 1 0.784314 rgBT /Overlock 10 25, 919-929.	2.0	10
48	A new CPA equation of state for water and primary alcohols. Physics and Chemistry of Liquids, 2014, 52, 701-709.	1.2	2
49	Activity coefficient of monomer in different aggregates of a surfactant solution: a Lattice Monte Carlo Study. Journal of the Iranian Chemical Society, 2013, 10, 379-383.	2.2	1
50	Conductometric studies of thermodynamics of complexation of Li+, Na+ and K+ ions with 4â€²,4â€³(5â€³)-di-tert-butyldibenzo-18-crown-6 in binary acetonitrileâ€“nitromethane mixtures. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 77, 375-383.	1.6	5
51	Conductometric Studies of Thermodynamics of 1,10-Didecyl-1,10-diaza-18-crown-6 Complexes with , , , , , , and Ions in Acetonitrile, Methanol, and Ethanol Solutions. Journal of Chemistry, 2013, 2013, 1-9.	1.9	3
52	On the Difference between Self-Assembling Process of Monomeric and Dimeric Surfactants with the Same Head to Tail Ratio: A Lattice Monte Carlo Simulation. Journal of Chemistry, 2013, 2013, 1-7.	1.9	3
53	Multinuclear magnetic resonance study of N-phenyl-aza-15-crown-5 complexes with lithium, sodium and caesium ions in nonaqueous solvents. Physics and Chemistry of Liquids, 2013, 51, 102-111.	1.2	3
54	Conductometric Studies of Thermodynamics of Complexation of Co2+, Ni2+, Cu2+, and Zn2+ Cations with Aza-18-crown-6 in Binary Acetonitrile-Methanol Mixtures. Journal of Thermodynamics, 2012, 2012, 1-10.	0.8	4

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55	Study on the interaction between dinaphthosulfide-substituted macrocyclic diamides and some metal ions: experimental measurements vs. quantum mechanical calculations. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2012, 73, 255-262.	1.6	4
56	Equation of state for polymers based on glass transition data. Colloid and Polymer Science, 2011, 289, 1081-1087.	2.1	10
57	Basis set effects on the prediction accuracy of relative acidity constants of primary and secondary amines. Computational and Theoretical Chemistry, 2011, 966, 54-61.	2.5	1
58	Prediction of relative pK a values of amines by quantum chemical calculations. Monatshefte FÃ¼r Chemie, 2010, 141, 1195-1202.	1.8	2
59	Cavity shape effect on pKa prediction of small amines. Computational and Theoretical Chemistry, 2009, 910, 99-103.	1.5	11
60	Individual and simultaneous determinations of phenothiazine drugs using PCR, PLS and (OSC)-PLS multivariate calibration methods. Journal of the Serbian Chemical Society, 2008, 73, 233-247.	0.8	13
61	Monte Carlo Simulation of Microemulsion Phase Transitions by Solvent Accessible Surface Area. Journal of the Chinese Chemical Society, 2008, 55, 716-723.	1.4	2
62	Simultaneous Kineticâ€Spectrophotometric Determination of Hydrazine and its Derivatives by Partial Least Squares and Principle Component Regression Methods. Journal of the Chinese Chemical Society, 2007, 54, 15-21.	1.4	6