Hakan Kayi

List of Publications by Year
in descending order

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34	373	758635 12	839053 18
papers	citations	h-index	g-index

34	34	34	432
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	AM1* parameters for copper and zinc. Journal of Molecular Modeling, 2007, 13, 965-979.	0.8	35
2	Stimuli-responsive properties of aminophenylboronic acid-carrying thermosensitive copolymers. Polymer International, 2003, 52, 649-657.	1.6	30
3	A theoretical investigation of the relative stability of hydrated glycine and methylcarbamic acidâ€"from water clusters to interstellar ices. Physical Chemistry Chemical Physics, 2012, 14, 4942.	1.3	25
4	AM1* parameters for bromine and iodine. Journal of Molecular Modeling, 2009, 15, 295-308.	0.8	22
5	Ni(II), Cu(II), and Zn(II) complexes of tetradentate schiff base containing two thiadiazoles units: Structural, spectroscopic, magnetic properties, and molecular modeling studies. Heteroatom Chemistry, 2008, 19, 700-712.	0.4	21
6	A computational study on the structures of methylamineâ€"carbon dioxideâ€"water clusters: evidence for the barrier free formation of the methylcarbamic acid zwitterion (CH3NH2+COOâ^') in interstellar water ices. Physical Chemistry Chemical Physics, 2011, 13, 11083.	1.3	21
7	AM1* parameters for cobalt and nickel. Journal of Molecular Modeling, 2010, 16, 29-47.	0.8	18
8	Kinetics of CO 2 capture by carbon dioxide binding organic liquids: Experimental and molecular modelling studies. International Journal of Greenhouse Gas Control, 2016, 49, 379-386.	2.3	18
9	A theoretical investigation of the low energy conformers of the isomers glycine and methylcarbamic acid and their role in the interstellar medium. Physical Chemistry Chemical Physics, 2011, 13, 15774.	1.3	17
10	Pseudo Jahnâ€"Teller origin of bending instability of triatomic molecules. Journal of Molecular Structure, 2012, 1023, 108-114.	1.8	16
11	Deviations from Bornâ€"Oppenheimer Theory in Structural Chemistry: Jahnâ€"Teller, Pseudo Jahnâ€"Teller, and Hidden Pseudo Jahnâ€"Teller Effects in C₃H₃ and C₃H₃^{â€"}. Journal of Physical Chemistry A, 2013, 117, 8671-8679.	1.1	16
12	AM1* parameters for vanadium and chromium. Journal of Molecular Modeling, 2009, 15, 1253-1269.	0.8	15
13	Prediction of lower critical solution temperature of N-isopropylacrylamideâ€"acrylic acid copolymer by an artificial neural network model. Journal of Molecular Modeling, 2005, 11, 55-60.	0.8	12
14	AM1* parameters for manganese and iron. Journal of Molecular Modeling, 2010, 16, 1109-1126.	0.8	12
15	Conformational behaviors of trans-2,3- and trans-2,5-dihalo-1,4-diselenanes. A complete basis set, hybrid-density functional theory study and natural bond orbital interpretations. Journal of Molecular Modeling, 2014, 20, 2249.	0.8	9
16	A computational study on 4,7-di(furan-2-yl)benzo[c][1,2,5]thiadiazole monomer and its oligomers. Journal of Molecular Modeling, 2014, 20, 2269.	0.8	9
17	Innovative Carbon Dioxideâ€Capturing Organic Solvent: Reaction Mechanism and Kinetics. Chemical Engineering and Technology, 2017, 40, 737-744.	0.9	8
18	AM1* parameters for gold. Journal of Molecular Modeling, 2010, 16, 1029-1038.	0.8	7

#	Article	IF	Citations
19	AM1* parameters for palladium and silver. Journal of Molecular Modeling, 2011, 17, 2585-2600.	0.8	7
20	Natural bond orbital, nuclear magnetic resonance analysis and hybrid-density functional theory study of Ïƒ-aromaticity in Al2F6, Al2Cl6, Al2Br6 and Al2I6. Journal of Molecular Modeling, 2013, 19, 2549-2557.	0.8	7
21	A theoretical investigation of 4,7-di(furan-2-yl)benzo[c][1,2,5]selenadiazole-based donorâ€“acceptor type conjugated polymer. Computational and Theoretical Chemistry, 2015, 1054, 38-45.	1.1	7
22	Monodisperse-porous cerium oxide microspheres as a new support with appreciable catalytic activity for a composite catalyst in benzyl alcohol oxidation. New Journal of Chemistry, 2021, 45, 2019-2029.	1.4	6
23	Capture of Carbonyl Sulfide by Organic Liquid Mixtures: A Systematic DFT Investigation. Industrial & Engineering Chemistry Research, 2021, 60, 1366-1374.	1.8	6
24	Monodisperse-porous cerium oxide microspheres carrying iridium oxide nanoparticles as a heterogeneous catalyst for water oxidation. Applied Surface Science, 2021, 547, 149219.	3.1	6
25	Experimental and theoretical investigation of the reaction between CO$_{2}$ and carbon dioxide binding organic liquids. Turkish Journal of Chemistry, 2016, 40, 706-719.	0.5	4
26	Design of novel tellurium and selenium containing semiconducting polymers using quantum mechanical tools. Computational and Theoretical Chemistry, 2017, 1099, 45-54.	1.1	4
27	Radicalic cleavage pathway and DNA docking studies of novel chemotherapic platinum agent of 5,6-di-2-ithienyl-2,3-dihydropyrazine. Polyhedron, 2019, 170, 25-33.	1.0	4
28	Spectroelectrochemical Investigation of Nuclease Active Pt(II) Complexes Containing Pyrrole Oximeâ€. Electrochimica Acta, 2015, 158, 333-341.	2.6	3
29	Correlations between hardness, electrostatic interactions, and thermodynamic parameters in the decomposition reactions of 3-buten-1-ol, 3-methoxy-1-propene, and ethoxyethene. Structural Chemistry, 2015, 26, 547-554.	1.0	3
30	Anticancer investigation of platinum and copper-based complexes containing quinoxaline ligands. Journal of Molecular Structure, 2022, 1250, 131928.	1.8	3
31	Effect of chalcogen atoms on the electronic band gaps of donor-acceptor-donor type semiconducting polymers: a systematic DFT investigation. Journal of Molecular Modeling, 2019, 25, 167.	0.8	2
32	Kinetics of CO2 Capture by Carbon Dioxide Binding Organic Liquids. Green Energy and Technology, 2016, , 591-603.	0.4	0
33	Artificial Neural Network Prediction of Sulfur Content of Diesel fuel from its Physical Properties. IOP Conference Series: Materials Science and Engineering, 2019, 518, 062008.	0.3	0
34	Theoretical investigation of carbon dioxide capture by aqueous boric acid solution: A termolecular reaction mechanism. Journal of Boron, 0, , .	0.0	0