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List of Publications by Year
in descending order

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88 papers	1,359 citations	361413 20 h-index	434195 31 g-index
88 all docs	88 docs citations	88 times ranked	1526 citing authors

#	Article	IF	Citations
1	A binuclear copper(II) complex based on hydrazone ligand: Characterization, molecular docking, and theoretical and antimicrobial investigation. Applied Organometallic Chemistry, 2022, 36, e6461.	3.5	7
2	Are metal dopant and ligands efficient to optimize the adsorption rate of CH4, H2 and H2S on IRMOFs? Insights from factorial design. Computational Materials Science, 2022, 210, 111438.	3.0	5
3	Organometallic gold (III) and platinum (II) complexes with thiosemicarbazone: Structural behavior, anticancer activity, and molecular docking. Applied Organometallic Chemistry, 2022, 36, .	3.5	5
4	IRMOF â€8: Theoretical evaluation of aluminum doping on hydrogen, methane, and hydrogen sulfide adsorption. International Journal of Quantum Chemistry, 2021, 121, e26510.	2.0	6
5	Theoretical evaluation of the performance of IRMOFs and M-MOF-74 in the formation of 5-fluorouracil@MOF. RSC Advances, 2021, 11, 31090-31097.	3.6	11
6	Nature and role of the weak intermolecular bond in enantiomeric conformations of H₂O₂â€“noble gas adducts: a chiral prototypical model. New Journal of Chemistry, 2021, 45, 8240-8247.	2.8	3
7	Analysis of Conformational, Structural, Magnetic, and Electronic Properties Related to Antioxidant Activity: Revisiting Flavan, Anthocyanidin, Flavanone, Flavonol, Isoflavone, Flavone, and Flavan-3-ol. ACS Omega, 2021, 6, 8908-8918.	3.5	47
8	Investigation of strength and nature of the weak intermolecular bond in NH2 radical-noble gas atom adducts and evaluation of their basic spectroscopic features. Chemical Physics Letters, 2021, 769, 138386.	2.6	3
9	Electronic and structural study of T315I mutated form in DFG-out conformation of BCR-ABL inhibitors. Journal of Biomolecular Structure and Dynamics, 2021, , 1-15.	3.5	4
10	Removal of hydrogen sulfide from a binary mixture with methane gas, using IRMOF-1: a theoretical investigation. Journal of Molecular Modeling, 2021, 27, 240.	1.8	4
11	Investigation on the interaction behavior of afatinib, dasatinib, and imatinib docked to the BCR-ABL protein. Journal of Molecular Modeling, 2021, 27, 309.	1.8	4
12	DFT analysis, spectroscopic study and biological activity of a newly synthesized benzoylhydrazone binuclear Cu(II) complex. Journal of Inorganic Biochemistry, 2020, 204, 110949.	3.5	22
13	Accurate spectroscopic properties by diffusion quantum Monte Carlo calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 243, 118707.	3.9	0
14	Computational analysis of vibrational frequencies and rovibrational spectroscopic constants of hydrogen sulfide dimer using MP2 and CCSD(T). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118540.	3.9	14
15	Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr,) Tj ETQq1 1 0.784314 rgBT /O	2.5	5
16	High Coverage of H2, CH4, NH3 and H2O on (110) SnO2 Nanotubes. Engineering Materials, 2020, , 169-188.	0.6	0
17	Effect of Hubbard parameter and semi-empirical van der Waals correction on benzene adsorption over anatase TiO2 (1â€²0â€²1) surface. Computational and Theoretical Chemistry, 2019, 1164, 112552.	2.5	4
18	Analysis of lowest energy transitions at TD-DFT of pyrene in vacuum and solvent. Journal of Molecular Modeling, 2019, 25, 183.	1.8	14

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19	BTEX adsorption on TiO2 anatase and rutile surfaces: DFT functionals. Journal of Molecular Modeling, 2019, 25, 137.	1.8	8
20	Dynamics and spectroscopy of van der Waals complexes composed of ammonia and noble gases. Journal of Molecular Modeling, 2019, 25, 126.	1.8	0
21	Methanol, ethanol, propanol, and butanol adsorption on H-ZSM-5 zeolite: an ONIOM study. Journal of Molecular Modeling, 2019, 25, 34.	1.8	14
22	Similarity search combined with docking and molecular dynamics for novel hAChE inhibitor scaffolds. Journal of Molecular Modeling, 2018, 24, 41.	1.8	13
23	Interface Interactions of the Bowmanâ€“Birk Inhibitor BTCI in a Ternary Complex with Trypsin and Chymotrypsin Evaluated by Semiempirical Quantum Mechanical Calculations. European Journal of Organic Chemistry, 2018, 2018, 5203-5211.	2.4	5
24	Electronic structure of GaN nanotubes. Comptes Rendus Chimie, 2017, 20, 190-196.	0.5	20
25	Potential acetylcholinesterase inhibitors: molecular docking, molecular dynamics, and in silico prediction. Journal of Molecular Modeling, 2017, 23, 67.	1.8	24
26	Binding Analysis of Some Classical Acetylcholinesterase Inhibitors: Insights for a Rational Design Using Free Energy Perturbation Method Calculations with QM/MM MD Simulations. Journal of Chemical Information and Modeling, 2017, 57, 958-976.	5.4	28
27	Stability of rolled-up GaAs nanotubes. Journal of Molecular Modeling, 2017, 23, 204.	1.8	4
28	Quantum Monte Carlo with density matrix: potential energy curve derived properties. Journal of Molecular Modeling, 2017, 23, 104.	1.8	2
29	Simulations and Analysis of Titanium Dioxide Nanotubes (Rutile (110) and Anatase (101)). Current Physical Chemistry, 2016, 6, 10-21.	0.2	3
30	New Cu(II) complex with acetylpyridine benzoyl hydrazone: experimental and theoretical analysis. Journal of Coordination Chemistry, 2016, 69, 330-342.	2.2	10
31	Improving the Description of the Optical Properties of Carotenoids by Tuning the Long-Range Corrected Functionals. Journal of Physical Chemistry A, 2016, 120, 4944-4950.	2.5	32
32	CO₂ adsorption on single-walled boron nitride nanotubes containing vacancy defects. RSC Advances, 2015, 5, 27412-27420.	3.6	28
33	Lateral interaction and spectroscopic constants of CO adsorbed on ZnO. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	6
34	Rovibrational energies and spectroscopic constants for H2Oâ^'Ng complexes. Journal of Molecular Modeling, 2014, 20, 2498.	1.8	17
35	Structure and electronic properties of azadirachtin. Journal of Molecular Modeling, 2014, 20, 2084.	1.8	8
36	A detailed reactive cross section study of X + Li2 â†' Li + LiX, with X = H, D, T, and Mu. Journal of Molecular Modeling, 2014, 20, 2315.	1.8	4

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37	Investigation of the torsional barrier of EDOT using molecular mechanics and DFT methods. Journal of Molecular Modeling, 2014, 20, 2405.	1.8	2
38	Rovibrational energy and spectroscopic constant calculations of CH 4â€‰â‹¯â€‰CH 4, CH 4â€‰â‹¯â€‰H 2 O, CH 4â€‰â‹¯â€‰CHF H 2 Oâ€‰â‹¯â€‰CHF 3 dimers. Journal of Molecular Modeling, 2014, 20, 2298.	1.8	8
39	Relativistic Four-Component Potential Energy Curves for the Lowest 23 Covalent States of Molecular Bromine (Br₂). Journal of Physical Chemistry A, 2014, 118, 5818-5822.	2.5	12
40	Carbon dioxide adsorption on doped boron nitride nanotubes. RSC Advances, 2014, 4, 28249-28258.	3.6	34
41	Acetylcholinesterase inhibitors: Modeling potential candidates. International Journal of Quantum Chemistry, 2013, 113, 1461-1466.	2.0	6
42	Electronic and optical properties of BGO:Nd: The role of localized and delocalized f electrons. Chemical Physics Letters, 2013, 578, 76-80.	2.6	3
43	Vibrational and Electronic Structure Analysis of a Carbon Dioxide Interaction with Functionalized Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2013, 117, 2854-2861.	2.5	20
44	CO2 adsorption on polar surfaces of ZnO. Journal of Molecular Modeling, 2013, 19, 2069-2078.	1.8	23
45	The H + Li2 bimolecular exchange reaction: Dynamical and kinetical properties at J = 0. Journal of Chemical Physics, 2012, 136, 134319.	3.0	14
46	Theoretical study of disubstituted pyrrolopyrimidines as focal adhesion kinase inhibitors. International Journal of Quantum Chemistry, 2012, 112, 2324-2329.	2.0	3
47	Benzeneâ€“kaolinite interaction properties. International Journal of Quantum Chemistry, 2012, 112, 2828-2831.	2.0	9
48	ONIOM study of dissociated hydrogen and water on ZnO surface. International Journal of Quantum Chemistry, 2012, 112, 3223-3227.	2.0	10
49	Bonding and electronic structure of sillenites. Chemical Physics Letters, 2012, 533, 78-81.	2.6	15
50	Spectroscopic properties of the molecular ion in the 8kΪ€, 9kΪƒ, 9lΪ€, 9lΪƒ and 10oΪƒ electronic states. Journal of Molecular Spectroscopy, 2012, 273, 26-29.	1.2	13
51	A chromophoric study of 2-ethylhexyl p-methoxycinnamate. Chemical Physics Letters, 2011, 516, 162-165.	2.6	13
52	Electronic structure and PCA analysis of covalent and non-covalent acetylcholinesterase inhibitors. Journal of Molecular Modeling, 2011, 17, 1371-1379.	1.8	18
53	Dynamical properties and thermal rate coefficients for the Na + HF reaction using genetic algorithm. International Journal of Quantum Chemistry, 2010, 110, 1070-1079.	2.0	7
54	Thermal rate coefficients calculation for the H⁺ + LiH reaction. International Journal of Quantum Chemistry, 2010, 110, 2024-2028.	2.0	5

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55	A Computational Investigation of the Multiple Channels of the NF2 + F Reaction. Journal of Physical Chemistry A, 2009, 113, 14336-14342.	2.5	3
56	Theoretical investigation of carotenoid ultraviolet spectra. International Journal of Quantum Chemistry, 2009, 109, 739-745.	2.0	35
57	New potential AChE inhibitor candidates. European Journal of Medicinal Chemistry, 2009, 44, 3754-3759.	5.5	46
58	Single walled MgF2 nanotubes. Computational Materials Science, 2009, 46, 233-238.	3.0	11
59	Theoretical Study of CH4â˜CH4, CHF3â˜CH4, CH4â˜H2O, and CHF3â˜H2O Dimers. Journal of Physical Chemistry A, 2009, 113, 14818-14823.	2.5	30
60	Quantum reactive study of a potential energy surface obtained via genetic algorithm. International Journal of Quantum Chemistry, 2008, 108, 2306-2311.	2.0	1
61	Study of the structureâ€activity relationship for theoretical molecular descriptors using density functional theory and chemometric methods in cannabinoid metabolites. International Journal of Quantum Chemistry, 2008, 108, 2530-2539.	2.0	3
62	Theoretical study of classical acetylcholinesterase inhibitors. Chemical Physics Letters, 2008, 458, 285-289.	2.6	20
63	Electronic and Structural Properties of the (101Ì…0) and (112Ì…0) ZnO Surfaces. Journal of Physical Chemistry A, 2008, 112, 8958-8963.	2.5	83
64	Electronic structure calculations toward new potentially AChE inhibitors. Chemical Physics Letters, 2007, 446, 304-308.	2.6	14
65	Theoretical study of cytosineâ€“Mg complex. Chemical Physics Letters, 2006, 418, 264-267.	2.6	14
66	Complexes of water with the fluoromethanes. Chemical Physics Letters, 2006, 431, 51-55.	2.6	15
67	Theoretical Study of Benzene Interaction on Kaolinite. Journal of Computer-Aided Materials Design, 2006, 12, 121-129.	0.7	16
68	Interaction of pyridine on Nb2O5. Computational and Theoretical Chemistry, 2005, 732, 1-5.	1.5	10
69	Theoretical study of kaolinite. International Journal of Quantum Chemistry, 2005, 103, 550-556.	2.0	25
70	AnÃ¡lise teÃ³rica da interaÃ§Ã£o de CO, CO2 e NH3 com ZnO. Quimica Nova, 2004, 27, 10-16.	0.3	6
71	The interaction of H2, CO, CO2, H2O and NH3 on ZnO surfaces: an Oniom Study. Chemical Physics Letters, 2004, 400, 481-486.	2.6	70
72	Theoretical analysis of water coverage on MgO(001) surfaces with defects and without F, V and P type vacancies. Computational and Theoretical Chemistry, 2003, 664-665, 111-124.	1.5	6

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73	A theoretical analysis on electronic structure of the (110) surface of TiO2â€“SnO2 mixed oxide. Computational and Theoretical Chemistry, 2003, 629, 307-314.	1.5	16
74	Theoretical ab initio study of ranitidine. International Journal of Quantum Chemistry, 2002, 90, 575-586.	2.0	15
75	Theoretical analysis on TiO2(110)/*V* surface. International Journal of Quantum Chemistry, 2001, 85, 44-51.	2.0	10
76	Theoretical study of MgO(001) surfaces: Pure, doped with Fe, Ca, and Al, and with and without adsorbed water. International Journal of Quantum Chemistry, 2001, 84, 705-713.	2.0	13
77	Theoretical study of ZnO (1010) and Cu/ZnO (1010) surfaces. Chemical Physics Letters, 2001, 338, 224-230.	2.6	35
78	Lateral interaction of CO and H 2 molecules on ZnO surfaces: an AM1 study. Computational and Theoretical Chemistry, 2000, 528, 161-170.	1.5	23
79	Theoretical study of metiamide, a histamine H2 antagonist. International Journal of Quantum Chemistry, 1998, 69, 117-128.	2.0	11
80	CO2 and NH3 interaction with ZnO surface: An AM1 study. International Journal of Quantum Chemistry, 1998, 70, 367-374.	2.0	16
81	Ab initio and semiempirical studies of the adsorption and dissociation of water on pure, defective, and doped MgO (001) surfaces. Journal of Chemical Physics, 1998, 109, 3671-3685.	3.0	26
82	CO interaction with ZnO surfaces: an MNDO, AM1 and PM3 theoretical study with large cluster models. Computational and Theoretical Chemistry, 1996, 363, 249-256.	1.5	14
83	H2O and H2 interaction with ZnO surfaces: A MNDO, AM1, and PM3 theoretical study with large cluster models. International Journal of Quantum Chemistry, 1996, 57, 861-870.	2.0	42
84	A theoretical study of (1010) and (0001) ZnO surfaces: molecular cluster model, basis set and effective core potential dependence. Computational and Theoretical Chemistry, 1995, 330, 301-306.	1.5	28
85	A theoretical study of water adsorption on (10-10) and (0001) ZnO surfaces: molecular cluster, basis set and effective core potential dependence. Computational and Theoretical Chemistry, 1995, 330, 347-351.	1.5	44
86	Am1 and pm3 transition structure for the hydride transfer. A model of reaction catalyzed by dihydrofolate reductase. Computational and Theoretical Chemistry, 1995, 330, 411-416.	1.5	24
87	Theoretical study of cluster models and molecular hydrogen interaction with SnO2 [110] surface. Computational and Theoretical Chemistry, 1995, 335, 167-174.	1.5	16
88	Quantum chemical study of the adsorption of water on zinc oxide surface. Computational and Theoretical Chemistry, 1994, 303, 19-24.	1.5	19