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List of Publications by Year
in descending order

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Version: 2024-02-01

78 papers	987 citations	516710 16 h-index	552781 26 g-index
79 all docs	79 docs citations	79 times ranked	1071 citing authors

#	Article	IF	Citations
1	DFT+U study of the electronic structure changes of WO3 monoclinic and hexagonal surfaces upon Cu, Ag, and Au adsorption. Applications for CO adsorption. Surface Science, 2021, 714, 121907.	1.9	10
2	Conversion of methanol to dimethyl ether over silicoaluminophosphates: Isolated acid sites and the influence of silicon islands. A DFT-ONIOM study. Microporous and Mesoporous Materials, 2020, 292, 109732.	4.4	10
3	Periodic DFT study of water adsorption on m-WO3(001), m-WO3(100), h-WO3(001) and h-WO3(100). Role of hydroxyl groups on the stability of polar hexagonal surfaces. Surface Science, 2020, 694, 121558.	1.9	17
4	Discovering the root of the stability of hexagonal WO3 surfaces from a periodic DFT perspective. Applied Surface Science, 2020, 506, 144719.	6.1	13
5	DFT thermodynamic study of the adsorption of CO2 and H2O on W3Ox/M(1 1 1) (xâ€¯=â€¯6 or 9 and Mâ€¯=â€¯Cu, Ag) Tj ETQq1 1 0.78	6.1	11
6	Selective catalytic reduction of nitrogen oxide by ammonia over Cu/SAPO-11: a theoretical study. SN Applied Sciences, 2020, 2, 1.	2.9	5
7	New theoretical insight on the acid sites distribution, their local structures and acid strength of the SAPOâ€11 molecular sieve. International Journal of Quantum Chemistry, 2018, 118, e25541.	2.0	2
8	Advances in Theoretical Studies on Solid Catalysts for Renewable Energy Production. Advances in Chemical and Materials Engineering Book Series, 2018, , 1-32.	0.3	0
9	NO and NO 2 adsorption on subsurface doped MgO (100) and BaO (100) surfaces. A density functional study. Applied Surface Science, 2017, 404, 216-229.	6.1	12
10	Comparative theoretical study of Au1-3 and Cu1-3 clusters supported on SAPO-11 and their interactions with CO. Journal of Computational Methods in Sciences and Engineering, 2017, 17, 89-96.	0.2	1
11	On the Electronic Effect of V, Fe, and Ni on MgO(100) and BaO(100) Surface: An Explanation from a Periodic Density Functional. Journal of Chemistry, 2016, 2016, 1-8.	1.9	1
12	A reinvestigation of the CO vibration frequency as a probe to determine the species of Au in the Au/MOR catalyst. Applied Catalysis A: General, 2016, 526, 53-61.	4.3	4
13	MÃ¸llerâ€“Plesset 2 and density functional theory studies of the interaction between aromatic compounds and Zn-porphyrins. Computational and Theoretical Chemistry, 2016, 1084, 133-139.	2.5	3
14	Periodic DFT study of Ti deposition on defective Si(100) surfaces. Applied Surface Science, 2015, 335, 160-166.	6.1	1
15	HAl(OH)2 molecular structures and reaction paths. Post-Hartreeâ€“Fock, DFT calculations and infrared spectroscopic. Computational and Theoretical Chemistry, 2015, 1060, 31-35.	2.5	1
16	A simple method for the determination of the Tolman electronic parameter of different phosphorus containing ligands, by means of the average local ionization energy. Inorganica Chimica Acta, 2015, 436, 163-168.	2.4	16
17	Theoretical Study of the Adsorption of Alkylamines in H-Mordenite: The Role of Noncovalent Interactions. Journal of Physical Chemistry C, 2015, 119, 8112-8123.	3.1	12
18	Theoretical ONIOM2/DFT study of Pd/ZSM-5 catalyst: CO and NO adsorption. Journal of Computational Methods in Sciences and Engineering, 2014, 14, 121-130.	0.2	0

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19	Theoretical study of small clusters Au5-6 on Au/SAPO-11 catalysts and their interactions with CO. Journal of Computational Methods in Sciences and Engineering, 2014, 14, 45-52.	0.2	0
20	Density functional study of NO adsorption on undefected and oxygen defective Auâ€“BaO(100) surfaces. Applied Surface Science, 2014, 307, 165-171.	6.1	3
21	Theoretical study of CO adsorption and oxidation on Au3â€“5 clusters supported on silico-aluminophospates. Computational and Theoretical Chemistry, 2014, 1042, 69-83.	2.5	5
22	Role of the Siâ€“Si bond stability in the first stages of Ti diffusion on a Si(111) 2Ã—1 surface. A periodic DFT study. Applied Surface Science, 2013, 273, 496-501.	6.1	2
23	Evaluation of BrÃ¸nsted Sites Inside the H-MOR Employing NH₃: A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 5112-5117.	3.1	12
24	Performance of Density Functional Methods. Some Difficult Cases for Small Systems Containing Cu, Ag, or Au. Journal of Physical Chemistry A, 2013, 117, 2619-2628.	2.5	6
25	Nitrogen oxides and SO2 adsorption on Au/MOR catalyst: Adsorption sites, thermodynamic and vibrational frequencies. ONIOM study. Journal of Molecular Catalysis A, 2012, 363-364, 380-386.	4.8	3
26	Theoretical study of small clusters Au3-4 on Au/SAPO-11 catalysts and their interactions with CO. Journal of Computational Methods in Sciences and Engineering, 2012, 12, 391-396.	0.2	0
27	Direct catalytic decomposition of NO with Cuâ€“ZSM-5: A DFTâ€“ONIOM study. Journal of Molecular Catalysis A, 2011, 348, 55-62.	4.8	22
28	Synthesis, characterization and biological activity of trans-platinum(II) complexes with chloroquine. Journal of Inorganic Biochemistry, 2011, 105, 1684-1691.	3.5	34
29	Theoretical study of Au/SAPO-11 catalyst and its potential use in thiophene HDS. Journal of Molecular Catalysis A, 2010, 315, 28-34.	4.8	12
30	Theoretical study of the CO catalytic oxidation on Au/SAPOâ€11 zeolite. International Journal of Quantum Chemistry, 2010, 110, 2573-2582.	2.0	4
31	Interaction of CO Molecule with Au/MOR Catalyst: ONIOM-PM6 Study, Active Sites, Thermodynamic and Vibrational Frequencies. Journal of Physical Chemistry A, 2010, 114, 6870-6878.	2.5	15
32	Theoretical study of the water effect on CO adsorbed over Au/SAPO-11 catalysts. Journal of Computational Methods in Sciences and Engineering, 2009, 9, 281-287.	0.2	3
33	Theoretical study of substituted methyl mercury in gas phase and in solution. Journal of Computational Methods in Sciences and Engineering, 2009, 9, 167-173.	0.2	0
34	Stabilization of the (110) tetragonal zirconia surface by hydroxyl chemical transformation. Surface Science, 2009, 603, 2526-2531.	1.9	21
35	DFT-ONIOM study of Au/ZSM-5 catalyst: Active sites, thermodynamic and vibrational frequencies. Journal of Molecular Catalysis A, 2009, 301, 61-66.	4.8	9
36	Theoretical study of CO and H2O interaction on (110) and (101) Zirconia surfaces. Computational and Theoretical Chemistry, 2009, 900, 59-63.	1.5	8

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37	Improvement of scale factors for harmonic vibrational frequency calculations using new polarization functions. International Journal of Quantum Chemistry, 2008, 108, 1036-1043.	2.0	16
38	Influence of isomorphous substitution on NO and N₂O thermochemistry on Au/ZSMâ€5 catalyst. International Journal of Quantum Chemistry, 2008, 108, 1696-1704.	2.0	5
39	Structural Transformation of (110) Ultrathin Films of Tetragonal Zirconia Induced by Polarity. Journal of Physical Chemistry C, 2007, 111, 8314-8320.	3.1	3
40	An ab initio and DFT study of the interaction between ethanethiol and zeolites. Journal of Molecular Catalysis A, 2007, 278, 165-172.	4.8	15
41	Synthesis and characterization of [Au(dppz)2]Cl3. DNA interaction studies and biological activity against Leishmania (L) mexicana. Journal of Inorganic Biochemistry, 2007, 101, 111-116.	3.5	71
42	ONIOM study of Ga/SAPO-11 catalyst: Species formation and reactivity. Journal of Molecular Catalysis A, 2007, 271, 185-191.	4.8	9
43	Theoretical Study on Silver- and Gold-Loaded Zeolite Catalysts:Â Thermodynamics and IR Spectroscopy. Journal of Physical Chemistry B, 2006, 110, 17912-17917.	2.6	11
44	Theoretical study of the mechanisms for the homogenous gas-phase elimination kinetics of some 2-hydroxynitroalkanes. Journal of Physical Organic Chemistry, 2006, 19, 836-840.	1.9	2
45	DFT Study of substituent effects of 2-substituted alkyl ethyl methylcarbonates in homogeneous, unimolecular gas phase elimination kinetics. International Journal of Chemical Kinetics, 2006, 38, 184-193.	1.6	9
46	Theoretical study of catalytic steam cracking on a asphaltene model molecule. Journal of Molecular Catalysis A, 2005, 227, 223-229.	4.8	27
47	Density functional theory calculation for H2 dissociation on MoS2 and NiMoS cluster models. Computational and Theoretical Chemistry, 2005, 729, 91-97.	1.5	7
48	Diatomic molecule data for parametric methods. I. Computational and Theoretical Chemistry, 2005, 729, 19-37.	1.5	39
49	Density functional study of the interaction of Cu+ ion-exchanged zeolites with H2O and SO2 molecules. Journal of Molecular Catalysis A, 2005, 228, 203-210.	4.8	17
50	Application of computational methods to catalytic systems. Journal of Molecular Catalysis A, 2005, 228, 211-225.	4.8	11
51	Theoretical study of the Ga/SAPO-11 catalyst. Journal of Molecular Catalysis A, 2005, 242, 233-240.	4.8	3
52	Theoretical study of beryllium (II) complexes using CATIVIC: New parametric method. International Journal of Quantum Chemistry, 2004, 97, 854-864.	2.0	9
53	Robust hydrogen-bonded self-assemblies from biimidazole complexes. Synthesis and structural characterization of [M(biimidazole)2(OH2)2]2+(M = Co2+, Ni2+) complexes and carboxylate modules. Dalton Transactions, 2004, , 505-513.	3.3	65
54	Theoretical calculations of silica supported Mo2(Î·3-C3H5)4 species. Computational and Theoretical Chemistry, 2003, 625, 59-70.	1.5	7

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55	Modeling MoS2 catalytic surface with simple clusters. Journal of Molecular Catalysis A, 2003, 192, 203-216.	4.8	11
56	Theoretical Study of the Interaction of NO2Molecule with a Metalâ"Zeolite Model (Metal = Cu, Ag, Au). Journal of Physical Chemistry A, 2002, 106, 6851-6856.	2.5	14
57	Theoretical Study of NO2 Adsorption on a Transition-Metal Zeolite Model. Journal of Catalysis, 2002, 205, 107-114.	6.2	37
58	Interaction of H2S with the X/MoS2Surface (X = Zn, Cu, Ni, Co). A Theoretical Study. Journal of Physical Chemistry A, 2001, 105, 6519-6525.	2.5	10
59	Parametric calculations of Mo-allyl complexes anchored on silica. Journal of Molecular Catalysis A, 2001, 168, 265-277.	4.8	5
60	Analysis of parametric functionals in semiempirical approaches using simulation techniques. Computational and Theoretical Chemistry, 1999, 469, 177-190.	1.5	20
61	Simulation Techniques in Parametric Hamiltonians. Journal of Chemical Information and Computer Sciences, 1999, 39, 543-549.	2.8	20
62	Topology of electronic densities taken from parametric methods: A predictive tool?. International Journal of Quantum Chemistry, 1998, 70, 113-123.	2.0	11
63	Diatomic interaction energies in the topological theory of atoms in molecules. Theoretica Chimica Acta, 1997, 95, 1-12.	0.8	6
64	Model parametric Hamiltonians and bonding theoretical tools in simulation of catalytic reaction steps. Hydrotreatment of oil components. Journal of Molecular Catalysis A, 1997, 119, 335-348.	4.8	14
65	Topological analysis of electron density distribution taken from a pseudopotential calculation. Journal of Computational Chemistry, 1997, 18, 416-429.	3.3	55
66	Diatomic interaction energies in the topological theory of atoms in molecules. Theoretica Chimica Acta, 1997, 95, 1.	0.8	16
67	Atomization of vanadium in a graphite furnace: experimental and theoretical modelling of surface interactions. Journal of Analytical Atomic Spectrometry, 1996, 11, 445.	3.0	13
68	The Laplacian of the electronic density at the valence-shell charge concentration (VSCC): A comparative study of effective core potential and full-electron calculations in Mo compounds. II. International Journal of Quantum Chemistry, 1996, 60, 1015-1026.	2.0	9
69	Modelling carbon chemisorption on a nickel catalyst. MINDOSR semiempirical calculations. Journal of Molecular Catalysis A, 1996, 106, 109-118.	4.8	8
70	H2 interaction with S atoms of a MoS2 modelled catalytic site: electronic density analysis for Sî—¸H formation. Journal of Molecular Catalysis A, 1996, 109, 227-238.	4.8	20
71	Bond functions and the topological properties of the bonds. Structural Chemistry, 1995, 6, 333-337.	2.0	0
72	Electronic density topology of metalâ€"metal quadruple bond in some Mo complexes. Chemical Physics Letters, 1994, 227, 557-560.	2.6	10

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73	A comparative study of effective core potential and full-electron calculations in Mo compounds. I. An analysis of topological properties of bond charge distribution. Journal of Computational Chemistry, 1994, 15, 313-321.	3.3	26
74	Chemistry of carbonizationâ€"I. A theoretical study of free radical formation from starting materials. Carbon, 1993, 31, 645-650.	10.3	8
75	Experimental and theoretical studies of the factors that influence the determination of molybdenum by electrothermal atomic absorption spectroscopy. Analytical Chemistry, 1993, 65, 1107-1113.	6.5	32
76	Theoretical modelling of molybdenum interaction with a graphite furnace surface. Computational and Theoretical Chemistry, 1992, 254, 387-393.	1.5	10
77	Quantum Mechanical Calculations of Chemical Interactions on Transition Metal Surfaces. , 1992, , 253-359.		3
78	Necessary conditions for the mapping ofÎ³intoÏ• Physical Review A, 1985, 32, 19-25.	2.5	24