Ewa Broclawik

List of Publications by Year
in descending order

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92	1,734	257101 24	329751 37
papers	citations	h-index	g-index

93	93	93	1729
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electronic Structure of Selected {FeNO}⁷ Complexes in Heme and Non-Heme Architectures: A Density Functional and Multireference ab Initio Study. Journal of Physical Chemistry B, 2010, 114, 1518-1528.	1.2	147
2	Time-dependent DFT study on electronic states of vanadium and molybdenum oxide molecules. Chemical Physics Letters, 2001, 339, 433-437.	1.2	88
3	DFT and Ab Initio Study of Iron-Oxo Porphyrins: May They Have a Low-Lying Iron(V)-Oxo Electromer?. Journal of Chemical Theory and Computation, 2011, 7, 898-908.	2.3	71
4	Study of the Activity of Ga-ZSM-5 in the de-NOx Process by a Combination of Quantum Chemistry, Molecular Dynamics, and Computer Graphics Methods. The Journal of Physical Chemistry, 1995, 99, 12461-12465.	2.9	58
5	Density functional theory calculations of the reaction pathway for methane activation on a gallium site in metal exchanged ZSMâ€5. Journal of Chemical Physics, 1995, 103, 2102-2108.	1.2	57
6	The role of tungsten in formation of active sites for no SCR on the V-W-O catalyst surface â€" quantum chemical modeling (DFT). Journal of Molecular Catalysis A, 2001, 166, 31-38.	4.8	42
7	Role of Substrate Positioning in the Catalytic Reaction of 4-Hydroxyphenylpyruvate Dioxygenaseâ€"A QM/MM Study. Journal of the American Chemical Society, 2014, 136, 14472-14485.	6.6	41
8	On the electronic structure of the palladium monoxide and the methane adsorption: Density functional calculations. Journal of Chemical Physics, 1996, 104, 4098-4104.	1.2	40
9	Density functional study on the activation of methane over Pd2, PdO, and Pd2O clusters. International Journal of Quantum Chemistry, 1997, 61, 673-682.	1.0	40
10	The distribution of framework aluminum atoms and extraframework exchanged cations in faujasite as studied by molecular dynamics, NMR simulation, neutron diffraction simulation and computer graphics. Microporous Materials, 1996, 7, 235-242.	1.6	39
11	Different support effect of M/ZrO2 and M/CeO2 (M=Pd and Pt) catalysts on CO adsorption: A periodic density functional study. Catalysis Today, 2006, 111, 322-327.	2.2	38
12	Spin-State Energetics of Fe(III) and Ru(III) Aqua Complexes: Accurate ab Initio Calculations and Evidence for Huge Solvation Effects. Journal of Chemical Theory and Computation, 2016, 12, 1592-1605.	2.3	38
13	Peculiarities of the Electronic Structure of Cytochrome P450 Compound I:â€‰ CASPT2 and DFT Modeling. Journal of Chemical Theory and Computation, 2007, 3, 728-734.	2.3	36
14	Density functional theory and quantum chemistry: Metals and metal oxides. Journal of Molecular Catalysis, 1993, 82, 117-129.	1.2	35
15	Catalytic Reaction Mechanism of Lipoxygenase. A Density Functional Theory Study. Journal of Physical Chemistry B, 2003, 107, 4639-4646.	1.2	34
16	Electronic structure and adsorption properties of precious metals and their oxides: Density functional calculations. Journal of Molecular Catalysis A, 1997, 119, 35-44.	4.8	32
17	Mechanism for Cyclization Reaction by Clavaminic Acid Synthase. Insights from Modeling Studiesâ€. Biochemistry, 2007, 46, 3682-3691.	1.2	32
18	Three-dimensional quantitative structureâ€"activity relationship (3 D-QSAR) and docking studies on (benzothiazole-2-yl) acetonitrile derivatives as c-Jun N-terminal kinase-3 (JNK3) inhibitors. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 5917-5925.	1.0	31

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19	Nitrogen Monoxide Interaction with Cu(I) Sites in Zeolites X and Y: Quantum Chemical Calculations and IR Studies. Journal of Physical Chemistry C, 2008, 112, 17998-18010.	1.5	30
20	Conformational Stability and Spin States of Cobalt(II) Acetylacetonate: CASPT2 and DFT Study. Journal of Chemical Theory and Computation, 2009, 5, 1237-1244.	2.3	30
21	IR studies and DFT quantum chemical calculations concerning interaction of some organic molecules with Cu+ sites in zeolites. Comptes Rendus Chimie, 2005, 8, 491-508.	0.2	29
22	On the Catalytic Mechanism of (S)â€2â€Hydroxypropylphosphonic Acid Epoxidase (HppE): A Hybrid DFT Study. Chemistry - A European Journal, 2013, 19, 771-781.	1.7	27
23	Periodic density functional investigation of Lewis acid sites in zeolites: relative strength order as revealed from NH3 adsorption. Applied Surface Science, 2005, 246, 96-101.	3.1	26
24	Epimerization and desaturation by carbapenem synthase (CarC). A hybrid DFT study. Journal of Computational Chemistry, 2006, 27, 740-748.	1.5	25
25	A quantum chemical investigation of the ammonium radical. I. SCF-XÎ±-SW calculations of the electronic structure and Rydberg spectra. Chemical Physics, 1982, 66, 417-423.	0.9	24
26	On the electronic structure of transition-metal oxide cations:DFTCalculations for VO+ and MoO+. International Journal of Quantum Chemistry, 1995, 56, 779-785.	1.0	22
27	First Principle Calculations for the Non-Heme Iron Centers of Lipoxygenases:Â Geometrical and Spectral Properties. Journal of Physical Chemistry B, 2001, 105, 12212-12220.	1.2	22
28	Mechanism of Benzylic Hydroxylation by 4-Hydroxymandelate Synthase. A Computational Study. Biochemistry, 2012, 51, 9570-9580.	1.2	22
29	Molecular dynamics simulation of traction fluid molecules under EHL condition. Thin Solid Films, 1996, 281-282, 598-601.	0.8	21
30	Title is missing!. Topics in Catalysis, 2000, 11/12, 271-278.	1.3	21
31	IR and NMR Studies of the Status of Al and Acid Sites in Desilicated Zeolite Y. Molecules, 2020, 25, 31.	1.7	21
32	Formaldehyde activation by Cu(I) and Ag(I) sites in ZSM-5: ETS-NOCV analysis of charge transfer processes. Catalysis Today, 2011, 169, 45-51.	2.2	20
33	On the electronic structure of MoO: Spin-polarized density functional calculations of spectroscopic properties of low-lying quintet, triplet, and septet states. International Journal of Quantum Chemistry, 1994, 52, 1017-1026.	1.0	19
34	Why Cu+ in ZSM-5 framework is active in DeNO reactionâ€"quantum chemical calculations and IR studies. Catalysis Today, 2002, 75, 353-357.	2.2	19
35	Application of Similarity Matrices and Genetic Neural Networks in Quantitative Structureâ^'Activity Relationships of 2- or 4-(4-Methylpiperazino)pyrimidines:Â 5-HT2AReceptor Antagonists. Journal of Medicinal Chemistry, 2000, 43, 1901-1909.	2.9	18
36	Molecular mechanism of Câ€"H bond cleavage at transition metal oxide clusters. Chemical Physics Letters, 2001, 333, 332-336.	1.2	18

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37	First-Principles Study on Proton Dissociation Properties of Fluorocarbon- and Hydrocarbon-Based Membranes in Low Humidity Conditions. Journal of Physical Chemistry B, 2006, 110, 17872-17877.	1.2	18
38	Electronic view on ethene adsorption in Cu(i) exchanged zeolites. Physical Chemistry Chemical Physics, 2010, 12, 2321.	1.3	17
39	Câ•€, Câ‰¡C, and Câ•Ο Bond Activation by Coinage Metal Cations in ZSM-5 Zeolites: Quantitative Charge Transfer Resolution. Journal of Physical Chemistry C, 2013, 117, 7511-7518.	1.5	16
40	Ammonia-modified Co(<scp>ii</scp>) sites in zeolites: spin and electron density redistribution through the Co^{II}â€“NO bond. Physical Chemistry Chemical Physics, 2016, 18, 3716-3729.	1.3	16
41	SCF-SW-X$alpha; studies of octahedral clusters in molybdenum oxides *1I. Simple octahedra. Journal of Catalysis, 1978, 51, 380-385.	3.1	15
42	On the nature of spin- and orbital-resolved Cu+â€“NO charge transfer in the gas phase and at Cu(I) sites in zeolites. Structural Chemistry, 2012, 23, 1349-1356.	1.0	15
43	Potential Energy Surface and Dynamics of Pd/MgO(001) System as Investigated by Periodic Density Functional Calculations and Classical Molecular Dynamics Simulations. Japanese Journal of Applied Physics, 2000, 39, 4255-4260.	0.8	14
44	DFT quantum chemical modeling of the interaction of alkenes with Cu+ sites in zeolites. Catalysis Today, 2006, 114, 162-168.	2.2	14
45	Development of Hybrid Tight-Binding Quantum Chemical Molecular Dynamics Method and Its Application to Boron Implantation into Preamorphized Silicon Substrate. Japanese Journal of Applied Physics, 2006, 45, 2970-2974.	0.8	14
46	From Electron Density Flow Towards Activation: Benzene Interacting with Cu(I) and Ag(I) Sites in ZSM-5. DFT Modeling. Catalysis Letters, 2008, 126, 241-246.	1.4	14
47	Torsionally Controlled Electronic Coupling in Mixed-Valence Oxodimolybdenum Nitrosyl Scorpionates - a DFT Study. Inorganic Chemistry, 2010, 49, 7676-7684.	1.9	14
48	Mechanisms of reactions conducted on Î±-amido-Î±-aminonitrones, determined based on the structures of their crystalline products and DFT calculations. New Journal of Chemistry, 2010, 34, 2220.	1.4	14
49	Nature of Copper Active Sites in CuZSM-5: Theory and Experiment. International Journal of Molecular Sciences, 2002, 3, 435-444.	1.8	13
50	First-principle calculations for the active centers in vanadium-containing chloroperoxidase and its functional models: Geometrical and spectral properties. International Journal of Quantum Chemistry, 2004, 99, 864-875.	1.0	13
51	Nitric oxide as a non-innocent ligand in (bio-)inorganic complexes: Spin and electron transfer in FeIINO bond. Journal of Inorganic Biochemistry, 2014, 136, 147-153.	1.5	13
52	Quintet electronic states of MoO: Gaussian density functional calculations. International Journal of Quantum Chemistry, 1992, 44, 393-399.	1.0	12
53	Simulation of AFM/LFM by molecular dynamics: role of lateral force in contact-mode AFM imaging. Surface Science, 1996, 357-358, 222-227.	0.8	12
54	Quantum chemical studies for oxidation of morpholine by Cytochrome P450. Journal of Inorganic Biochemistry, 2009, 103, 20-27.	1.5	12

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55	Mono- and Dinitrosyls on Copper(I) Site in a Zeolite Model: Effects of Static Correlation. Journal of Physical Chemistry A, 2011, 115, 11761-11774.	1.1	12
56	The electronic structure of the trisulfur trinitride anion. Inorganica Chimica Acta, 1983, 77, L101-L104.	1.2	10
57	Finite supercluster model of vanadium oxide catalysts. Journal of Molecular Catalysis, 1991, 68, 223-236.	1.2	9
58	Atomic Control of Ultrafine Gold Particles on MgO(100) as Investigated by Molecular Dynamics and Computer Graphics. Japanese Journal of Applied Physics, 1995, 34, 6873-6877.	0.8	9
59	Quantum chemical study on SiO desorption from a Si(111) surface. Surface Science, 1997, 387, 59-68.	0.8	9
60	Electronic propensity of Cu(II) versus Cu(I) sites in zeolites to activate NO â€" Spin- and orbital-resolved Cuâ€"NO electron transfer. Canadian Journal of Chemistry, 2013, 91, 538-543.	0.6	9
61	Tight-Binding Quantum Chemical Molecular Dynamics Study on Depth Profile Prediction in Low Energy Boron Implantation Process. Japanese Journal of Applied Physics, 2005, 44, 2288-2293.	0.8	8
62	The mechanism of the reaction of intradiol dioxygenase with hydroperoxy probe. Catalysis Today, 2011, 169, 207-216.	2.2	8
63	Theoretical estimation of acidâ€"base properties of Lewis and BrÃ¸nsted centres at the V-W-O catalyst surface: water molecule as the probe in DFT calculations. Journal of Molecular Catalysis A, 2004, 215, 187-193.	4.8	7
64	Hyperconjugation with lone pair of morpholine nitrogen stabilizes transition state for phenyl hydroxylation in CYP3A4 metabolism of (S)-N-[1-(3-morpholin-4-yl phenyl) ethyl]-3-phenylacrylamide. Chemical Physics Letters, 2006, 419, 523-527.	1.2	7
65	Cobalt cationic sites in ferrierites: QM/MM modeling. Catalysis Today, 2008, 137, 493-497.	2.2	7
66	Molecular dynamics study on the ligand recognition by tandem SH3 domains of p47phox, regulating NADPH oxidase activity. Computational Biology and Chemistry, 2006, 30, 303-312.	1.1	6
67	Oxidation mechanism in the metabolism of (S)-N-[1-(3-morpholin-4-ylphenyl)ethyl]-3-phenylacrylamide on oxyferryl active site in CYP3A4 Cytochrome: DFT modeling. Journal of Molecular Modeling, 2007, 13, 851-860.	0.8	6
68	The dependence on ammonia pretreatment of Nâ^'O activation by Co(II) sites in zeolites: a DFT and ab initio molecular dynamics study. Journal of Molecular Modeling, 2017, 23, 160.	0.8	6
69	Zeolites at the Molecular Level: What Can Be Learned from Molecular Modeling. Molecules, 2021, 26, 1511.	1.7	6
70	Cu+, Ag+ and Na+ Cationic Sites in ZSM-5 Interacting with Benzene: DFT Modeling. Studies in Surface Science and Catalysis, 2008, 174, 709-712.	1.5	5
71	Fine speciation of active sites in zeolites by a CO probe: Dynamics and IR frequencies. International Journal of Quantum Chemistry, 2018, 118, e25625.	1.0	5
72	On the ground electronic state of MoO+: Upgrade density functional theory calculations. Journal of Chemical Physics, 1999, 110, 11685-11687.	1.2	4

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73	Interaction of FeO⁺ cation with benzene, aniline, and 3â€methylaniline: DFT study of oxygen insertion mechanism. International Journal of Quantum Chemistry, 2008, 108, 2016-2022.	1.0	4
74	Theoretical modeling of electrochemical interactions in bimetallic molybdenum nitrosyl complexes incorporating saturated bridges. Polyhedron, 2008, 27, 2819-2824.	1.0	4
75	Ammonia-modified Co(<scp>ii</scp>) sites in zeolites: IR spectroscopy and spin-resolved charge transfer analysis of NO adsorption complexes. Physical Chemistry Chemical Physics, 2014, 16, 24089-24098.	1.3	4
76	A Theoretical Study of the Effect of Eu ion Dopant on the Electronic Excitations of Yttrium Oxide and Yttrium Oxy-Sulphide. Japanese Journal of Applied Physics, 2006, 45, 5782-5785.	0.8	3
77	A DFT Study of the Heme Role in the N-Demethylation of Theophylline Mediated by Compound I of Cytochrome P450. Materials Transactions, 2007, 48, 730-734.	0.4	3
78	Identity of two types of strong BrÃ¸nsted acid sites in mazzite revealed by CO probe: IR study and periodic DFT modeling. International Journal of Quantum Chemistry, 2019, 119, e25873.	1.0	3
79	Finite supercluster model of vanadium oxide catalysts. Part II. Adsorbateâ€"adsorbate interactions. Journal of Molecular Catalysis, 1993, 80, 341-352.	1.2	2
80	Characteristics of the ligandâ€"binding site interaction for a series of arecoline-derived muscarinic agonists: a quantum chemical study. Computers & Chemistry, 2000, 24, 411-420.	1.2	2
81	Quantum Chemical Calculations for some Toluene Derivatives. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1988, 43, 823-824.	0.7	1
82	Molecular simulation of the desorption process on solid surfaces under vacuum and supercritical conditions. Surface Science, 1996, 357-358, 703-707.	0.8	1
83	The role of the multi-body interaction in the de-NOx process on solid catalysts investigated by density functional method. Catalysis Today, 1997, 35, 189-196.	2.2	1
84	Theoretical Study on the ATP Hydrolysis Mechanism of HisP Protein, the ATP-Binding Subunit of ABC Transporter. Materials Transactions, 2007, 48, 735-739.	0.4	1
85	Does Metabolism of (<I>S</I>)-<I>N</I>-[1-(3-Morpholin-4-ylphenyl)ethyl]-3-phenylacrylamide Occur at the Morpholine Ring? Quantum Mechanical and Molecular Dynamics Studies. Materials Transactions, 2007, 48, 740-744.	0.4	1
86	Electronic Properties of Iron Sites and Their Active Forms in Porphyrin-Type Architectures. Springer Series on Bio- and Neurosystems, 2019, , 755-823.	0.2	1
87	Density Functional Theory as a Tool in Studying Catalytic Processes. Theoretical and Computational Chemistry, 1996, , 621-647.	0.2	0
88	Large-Scale Quantum Chemical Molecular Dynamics Simulations on the Formation Dynamics of Hydrogen by the Chemical Reactions of Water. , 2005, , 261.		0
89	Pharmacokinetic simulator with three-dimensional graphical models: Sociotechnological interface of pharmacokinetics for medical personnel, patients, and medicinal chemists. International Congress Series, 2005, 1284, 296-301.	0.2	0
90	Model first principles molecular dynamics study on the fate of vibrationally excited states in liquid water. Molecular Physics, 2006, 104, 2093-2100.	0.8	0

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91	Electronic structure of selenium chains by the SCF-SW-Xî± method. International Journal of Quantum Chemistry, 2009, 18, 395-403.	1.0	0
92	Particles of Biomedical Relevance and Their Interactions: A Classical and Quantum Mechanistic Approach to a Theoretical Description. , 2010, , 173-186.		0