

Ewa Broclawik

List of Publications by Year in descending order

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93
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docs citations

93
times ranked

1729
citing authors

#	ARTICLE	IF	CITATIONS
1	Zeolites at the Molecular Level: What Can Be Learned from Molecular Modeling. <i>Molecules</i> , 2021, 26, 1511.	1.7	6
2	IR and NMR Studies of the Status of Al and Acid Sites in Desilicated Zeolite Y. <i>Molecules</i> , 2020, 25, 31.	1.7	21
3	Identity of two types of strong Brønsted acid sites in mazzite revealed by CO probe: IR study and periodic DFT modeling. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25873.	1.0	3
4	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
5	Fine speciation of active sites in zeolites by a CO probe: Dynamics and IR frequencies. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25625.	1.0	5
6	The dependence on ammonia pretreatment of N ² O activation by Co(II) sites in zeolites: a DFT and ab initio molecular dynamics study. <i>Journal of Molecular Modeling</i> , 2017, 23, 160.	0.8	6
7	Spin-State Energetics of Fe(III) and Ru(III) Aqua Complexes: Accurate ab Initio Calculations and Evidence for Huge Solvation Effects. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1592-1605.	2.3	38
8	Ammonia-modified Co(II) sites in zeolites: spin and electron density redistribution through the Co ^{II} -NO bond. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3716-3729.	1.3	16
9	Nitric oxide as a non-innocent ligand in (bio-)inorganic complexes: Spin and electron transfer in FeII-NO bond. <i>Journal of Inorganic Biochemistry</i> , 2014, 136, 147-153.	1.5	13
10	Ammonia-modified Co(II) sites in zeolites: IR spectroscopy and spin-resolved charge transfer analysis of NO adsorption complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24089-24098.	1.3	4
11	Role of Substrate Positioning in the Catalytic Reaction of 4-Hydroxyphenylpyruvate Dioxygenase—A QM/MM Study. <i>Journal of the American Chemical Society</i> , 2014, 136, 14472-14485.	6.6	41
12	Electronic propensity of Cu(II) versus Cu(I) sites in zeolites to activate NO—Spin- and orbital-resolved Cu—NO electron transfer. <i>Canadian Journal of Chemistry</i> , 2013, 91, 538-543.	0.6	9
13	On the Catalytic Mechanism of (S)-2-Hydroxypropylphosphonic Acid Epoxidase (HppE): A Hybrid DFT Study. <i>Chemistry - A European Journal</i> , 2013, 19, 771-781.	1.7	27
14	C-C, C-C, and C-O Bond Activation by Coinage Metal Cations in ZSM-5 Zeolites: Quantitative Charge Transfer Resolution. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7511-7518.	1.5	16
15	Mechanism of Benzylic Hydroxylation by 4-Hydroxymandelate Synthase. A Computational Study. <i>Biochemistry</i> , 2012, 51, 9570-9580.	1.2	22
16	On the nature of spin- and orbital-resolved Cu+NO charge transfer in the gas phase and at Cu(I) sites in zeolites. <i>Structural Chemistry</i> , 2012, 23, 1349-1356.	1.0	15
17	DFT and Ab Initio Study of Iron-Oxo Porphyrins: May They Have a Low-Lying Iron(V)-Oxo Electromer?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 898-908.	2.3	71
18	Mono- and Dinitrosyls on Copper(I) Site in a Zeolite Model: Effects of Static Correlation. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11761-11774.	1.1	12

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19	Formaldehyde activation by Cu(I) and Ag(I) sites in ZSM-5: ETS-NOCV analysis of charge transfer processes. <i>Catalysis Today</i> , 2011, 169, 45-51.	2.2	20
20	The mechanism of the reaction of intradiol dioxygenase with hydroperoxy probe. <i>Catalysis Today</i> , 2011, 169, 207-216.	2.2	8
21	Torsionally Controlled Electronic Coupling in Mixed-Valence Oxodimolybdenum Nitrosyl Scorpionates - a DFT Study. <i>Inorganic Chemistry</i> , 2010, 49, 7676-7684.	1.9	14
22	Electronic Structure of Selected {FeNO} ⁷ Complexes in Heme and Non-Heme Architectures: A Density Functional and Multireference ab Initio Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1518-1528.	1.2	147
23	Electronic view on ethene adsorption in Cu(i) exchanged zeolites. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2321.	1.3	17
24	Mechanisms of reactions conducted on $\hat{\pm}$ -amido- $\hat{\pm}$ -aminonitrones, determined based on the structures of their crystalline products and DFT calculations. <i>New Journal of Chemistry</i> , 2010, 34, 2220.	1.4	14
25	Particles of Biomedical Relevance and Their Interactions: A Classical and Quantum Mechanistic Approach to a Theoretical Description. , 2010, , 173-186.		0
26	Electronic structure of selenium chains by the SCF-SW-X $\hat{\pm}$ method. <i>International Journal of Quantum Chemistry</i> , 2009, 18, 395-403.	1.0	0
27	Quantum chemical studies for oxidation of morpholine by Cytochrome P450. <i>Journal of Inorganic Biochemistry</i> , 2009, 103, 20-27.	1.5	12
28	Conformational Stability and Spin States of Cobalt(II) Acetylacetonate: CASPT2 and DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1237-1244.	2.3	30
29	From Electron Density Flow Towards Activation: Benzene Interacting with Cu(I) and Ag(I) Sites in ZSM-5. DFT Modeling. <i>Catalysis Letters</i> , 2008, 126, 241-246.	1.4	14
30	Interaction of FeO ⁺ cation with benzene, aniline, and 3- $\hat{\pm}$ -methylaniline: DFT study of oxygen insertion mechanism. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2016-2022.	1.0	4
31	Theoretical modeling of electrochemical interactions in bimetallic molybdenum nitrosyl complexes incorporating saturated bridges. <i>Polyhedron</i> , 2008, 27, 2819-2824.	1.0	4
32	Cobalt cationic sites in ferrierites: QM/MM modeling. <i>Catalysis Today</i> , 2008, 137, 493-497.	2.2	7
33	Nitrogen Monoxide Interaction with Cu(I) Sites in Zeolites X and Y: Quantum Chemical Calculations and IR Studies. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17998-18010.	1.5	30
34	Cu ⁺ , Ag ⁺ and Na ⁺ Cationic Sites in ZSM-5 Interacting with Benzene: DFT Modeling. <i>Studies in Surface Science and Catalysis</i> , 2008, 174, 709-712.	1.5	5
35	Theoretical Study on the ATP Hydrolysis Mechanism of HisP Protein, the ATP-Binding Subunit of ABC Transporter. <i>Materials Transactions</i> , 2007, 48, 735-739.	0.4	1
36	A DFT Study of the Heme Role in the N-Demethylation of Theophylline Mediated by Compound I of Cytochrome P450. <i>Materials Transactions</i> , 2007, 48, 730-734.	0.4	3

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37	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. <i>Materials Transactions</i> , 2007, 48, 740-744.	0.4	1
38	Mechanism for Cyclization Reaction by Clavaminc Acid Synthase. Insights from Modeling Studies. <i>Biochemistry</i> , 2007, 46, 3682-3691.	1.2	32
39	Peculiarities of the Electronic Structure of Cytochrome P450 Compound I: CASPT2 and DFT Modeling. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 728-734.	2.3	36
40	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. <i>Journal of Molecular Modeling</i> , 2007, 13, 851-860.	0.8	6
41	First-Principles Study on Proton Dissociation Properties of Fluorocarbon- and Hydrocarbon-Based Membranes in Low Humidity Conditions. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17872-17877.	1.2	18
42	Model first principles molecular dynamics study on the fate of vibrationally excited states in liquid water. <i>Molecular Physics</i> , 2006, 104, 2093-2100.	0.8	0
43	DFT quantum chemical modeling of the interaction of alkenes with Cu ⁺ sites in zeolites. <i>Catalysis Today</i> , 2006, 114, 162-168.	2.2	14
44	Molecular dynamics study on the ligand recognition by tandem SH3 domains of p47phox, regulating NADPH oxidase activity. <i>Computational Biology and Chemistry</i> , 2006, 30, 303-312.	1.1	6
45	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. <i>Chemical Physics Letters</i> , 2006, 419, 523-527.	1.2	7
46	Three-dimensional quantitative structure-activity relationship (3 D-QSAR) and docking studies on (benzothiazole-2-yl) acetonitrile derivatives as c-Jun N-terminal kinase-3 (JNK3) inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 5917-5925.	1.0	31
47	Different support effect of M/ZrO ₂ and M/CeO ₂ (M=Pd and Pt) catalysts on CO adsorption: A periodic density functional study. <i>Catalysis Today</i> , 2006, 111, 322-327.	2.2	38
48	Epimerization and desaturation by carbapenem synthase (CarC). A hybrid DFT study. <i>Journal of Computational Chemistry</i> , 2006, 27, 740-748.	1.5	25
49	Development of Hybrid Tight-Binding Quantum Chemical Molecular Dynamics Method and Its Application to Boron Implantation into Preamorphized Silicon Substrate. <i>Japanese Journal of Applied Physics</i> , 2006, 45, 2970-2974.	0.8	14
50	A Theoretical Study of the Effect of Eu ion Dopant on the Electronic Excitations of Yttrium Oxide and Yttrium Oxy-Sulphide. <i>Japanese Journal of Applied Physics</i> , 2006, 45, 5782-5785.	0.8	3
51	Periodic density functional investigation of Lewis acid sites in zeolites: relative strength order as revealed from NH ₃ adsorption. <i>Applied Surface Science</i> , 2005, 246, 96-101.	3.1	26
52	IR studies and DFT quantum chemical calculations concerning interaction of some organic molecules with Cu ⁺ sites in zeolites. <i>Comptes Rendus Chimie</i> , 2005, 8, 491-508.	0.2	29
53	Tight-Binding Quantum Chemical Molecular Dynamics Study on Depth Profile Prediction in Low Energy Boron Implantation Process. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 2288-2293.	0.8	8
54	Large-Scale Quantum Chemical Molecular Dynamics Simulations on the Formation Dynamics of Hydrogen by the Chemical Reactions of Water. , 2005, , 261.		0

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55	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
56	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
57	Theoretical estimation of acid-base properties of Lewis and Brønsted 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
58	Catalytic Reaction Mechanism of Lipoxygenase. A Density Functional Theory Study. Journal of Physical Chemistry B, 2003, 107, 4639-4646.	1.2	34
59	Nature of Copper Active Sites in CuZSM-5: Theory and Experiment. International Journal of Molecular Sciences, 2002, 3, 435-444.	1.8	13
60	Why Cu ⁺ in ZSM-5 framework is active in DeNO reaction—quantum chemical calculations and IR studies. Catalysis Today, 2002, 75, 353-357.	2.2	19
61	First Principle Calculations for the Non-Heme Iron Centers of Lipoxygenases: Geometrical and Spectral Properties. Journal of Physical Chemistry B, 2001, 105, 12212-12220.	1.2	22
62	The role of tungsten in formation of active sites for NO SCR on the V-W-O catalyst surface—quantum chemical modeling (DFT). Journal of Molecular Catalysis A, 2001, 166, 31-38.	4.8	42
63	Molecular mechanism of C-H bond cleavage at transition metal oxide clusters. Chemical Physics Letters, 2001, 333, 332-336.	1.2	18
64	Time-dependent DFT study on electronic states of vanadium and molybdenum oxide molecules. Chemical Physics Letters, 2001, 339, 433-437.	1.2	88
65	Characteristics of the ligand-binding site interaction for a series of arecoline-derived muscarinic agonists: a quantum chemical study. Computers & Chemistry, 2000, 24, 411-420.	1.2	2
66	Title is missing!. Topics in Catalysis, 2000, 11/12, 271-278.	1.3	21
67	Application of Similarity Matrices and Genetic Neural Networks in Quantitative Structure-Activity Relationships of 2- or 4-(4-Methylpiperazino)pyrimidines: 5-HT _{2A} Receptor Antagonists. Journal of Medicinal Chemistry, 2000, 43, 1901-1909.	2.9	18
68	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
69	On the ground electronic state of MoO ₄ ²⁺ : Upgrade density functional theory calculations. Journal of Chemical Physics, 1999, 110, 11685-11687.	1.2	4
70	Quantum chemical study on SiO desorption from a Si(111) surface. Surface Science, 1997, 387, 59-68.	0.8	9
71	The role of the multi-body interaction in the de-NO _x process on solid catalysts investigated by density functional method. Catalysis Today, 1997, 35, 189-196.	2.2	1
72	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

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73	Density functional study on the activation of methane over Pd ₂ , PdO, and Pd ₂ O clusters. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 673-682.	1.0	40
74	Simulation of AFM/LFM by molecular dynamics: role of lateral force in contact-mode AFM imaging. <i>Surface Science</i> , 1996, 357-358, 222-227.	0.8	12
75	Molecular simulation of the desorption process on solid surfaces under vacuum and supercritical conditions. <i>Surface Science</i> , 1996, 357-358, 703-707.	0.8	1
76	Density Functional Theory as a Tool in Studying Catalytic Processes. <i>Theoretical and Computational Chemistry</i> , 1996, , 621-647.	0.2	0
77	Molecular dynamics simulation of traction fluid molecules under EHL condition. <i>Thin Solid Films</i> , 1996, 281-282, 598-601.	0.8	21
78	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. <i>Microporous Materials</i> , 1996, 7, 235-242.	1.6	39
79	On the electronic structure of the palladium monoxide and the methane adsorption: Density functional calculations. <i>Journal of Chemical Physics</i> , 1996, 104, 4098-4104.	1.2	40
80	On the electronic structure of transition-metal oxide cations: DFT Calculations for VO ⁺ and MoO ⁺ . <i>International Journal of Quantum Chemistry</i> , 1995, 56, 779-785.	1.0	22
81	Atomic Control of Ultrafine Gold Particles on MgO(100) as Investigated by Molecular Dynamics and Computer Graphics. <i>Japanese Journal of Applied Physics</i> , 1995, 34, 6873-6877.	0.8	9
82	Density functional theory calculations of the reaction pathway for methane activation on a gallium site in metal exchanged ZSM-5. <i>Journal of Chemical Physics</i> , 1995, 103, 2102-2108.	1.2	57
83	Study of the Activity of Ga-ZSM-5 in the de-NO _x Process by a Combination of Quantum Chemistry, Molecular Dynamics, and Computer Graphics Methods. <i>The Journal of Physical Chemistry</i> , 1995, 99, 12461-12465.	2.9	58
84	On the electronic structure of MoO: Spin-polarized density functional calculations of spectroscopic properties of low-lying quintet, triplet, and septet states. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 1017-1026.	1.0	19
85	Density functional theory and quantum chemistry: Metals and metal oxides. <i>Journal of Molecular Catalysis</i> , 1993, 82, 117-129.	1.2	35
86	Finite supercluster model of vanadium oxide catalysts. Part II. Adsorbate-adsorbate interactions. <i>Journal of Molecular Catalysis</i> , 1993, 80, 341-352.	1.2	2
87	Quintet electronic states of MoO: Gaussian density functional calculations. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 393-399.	1.0	12
88	Finite supercluster model of vanadium oxide catalysts. <i>Journal of Molecular Catalysis</i> , 1991, 68, 223-236.	1.2	9
89	Quantum Chemical Calculations for some Toluene Derivatives. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 1988, 43, 823-824.	0.7	1
90	The electronic structure of the trisulfur trinitride anion. <i>Inorganica Chimica Acta</i> , 1983, 77, L101-L104.	1.2	10

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91	A quantum chemical investigation of the ammonium radical. I. SCF-X α -SW calculations of the electronic structure and Rydberg spectra. Chemical Physics, 1982, 66, 417-423.	0.9	24
92	SCF-SW-X α ; studies of octahedral clusters in molybdenum oxides *11. Simple octahedra. Journal of Catalysis, 1978, 51, 380-385.	3.1	15