Ariana Beste

List of Publications by Year
in descending order

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44 papers	1,592 citations	279487 23 h-index	288905 40 g-index
45 all docs	45 docs citations	45 times ranked	1763 citing authors

#	Article	IF	Citations
1	Computational Study of Bond Dissociation Enthalpies for Lignin Model Compounds. Substituent Effects in Phenethyl Phenyl Ethers. Journal of Organic Chemistry, 2009, 74, 2837-2841.	1.7	152
2	Direct Neutron Spectroscopy Observation of Cerium Hydride Species on a Cerium Oxide Catalyst. Journal of the American Chemical Society, 2017, 139, 9721-9727.	6.6	138
3	Computational Study of Bond Dissociation Enthalpies for Substituted Î²â€Oâ€4 Lignin Model Compounds. ChemPhysChem, 2011, 12, 3556-3565.	1.0	91
4	Density Functional Theory Study of the Concerted Pyrolysis Mechanism for Lignin Models. Energy & Fuels, 2014, 28, 5229-5235.	2.5	80
5	Computational study of bond dissociation enthalpies for lignin model compounds: Î²-5 Arylcoumaran. Chemical Physics Letters, 2012, 545, 100-106.	1.2	73
6	Computational Prediction of Î±/Î² Selectivities in the Pyrolysis of Oxygen-Substituted Phenethyl Phenyl Ethers. Journal of Physical Chemistry A, 2008, 112, 4982-4988.	1.1	72
7	ReaxFF Study of the Oxidation of Lignin Model Compounds for the Most Common Linkages in Softwood in View of Carbon Fiber Production. Journal of Physical Chemistry A, 2014, 118, 803-814.	1.1	68
8	Substituent Effects on the Reaction Rates of Hydrogen Abstraction in the Pyrolysis of Phenethyl Phenyl Ethers. Energy & Fuels, 2010, 24, 2857-2867.	2.5	65
9	Kinetic Analysis of the Pyrolysis of Phenethyl Phenyl Ether:â€‰Computational Prediction of Î±/Î²-Selectivities. Journal of Physical Chemistry A, 2007, 111, 12118-12126.	1.1	64
10	Adsorption and dissociation of methanol on the fully oxidized and partially reduced (111) cerium oxide surface: Dependence on the configuration of the cerium 4f electrons. Surface Science, 2008, 602, 162-175.	0.8	61
11	Pyrolysis Pathways of Sulfonated Polyethylene, an Alternative Carbon Fiber Precursor. Journal of the American Chemical Society, 2013, 135, 6130-6141.	6.6	60
12	Kinetic Analysis of the Phenyl-Shift Reaction in Î²-O-4 Lignin Model Compounds: A Computational Study. Journal of Organic Chemistry, 2011, 76, 2195-2203.	1.7	51
13	The Lewis Basicity of Diaminocarbene â€“ A Theoretical Study of Donorâ€“Acceptor Complexes of C(NH2)2, NH3 and CO with the Lewis Acids EF3, ECl3 (E = B, Al, Ga, In), TiF4 and TiCl4. European Journal of Inorganic Chemistry, 1999, 1999, 2037-2045.	1.0	46
14	Pathways for Ethanol Dehydrogenation and Dehydration Catalyzed by Ceria (111) and (100) Surfaces. Journal of Physical Chemistry C, 2015, 119, 2447-2455.	1.5	46
15	Role of Carbonâ€“Carbon Phenyl Migration in the Pyrolysis Mechanism of Î²-O-4 Lignin Model Compounds: Phenethyl Phenyl Ether and Î±-Hydroxy Phenethyl Phenyl Ether. Journal of Physical Chemistry A, 2012, 116, 12242-12248.	1.1	45
16	Kinetic simulation of the thermal degradation of phenethyl phenyl ether, a model compound for the Î²-O-4 linkage in lignin. Chemical Physics Letters, 2012, 550, 19-24.	1.2	40
17	ReaxFF Study of the Oxidation of Softwood Lignin in View of Carbon Fiber Production. Energy & Fuels, 2014, 28, 7007-7013.	2.5	37
18	Origins and implications of the ordering of oxygen vacancies and localized electrons on partially reduced<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CeO</mml:mi><mml:mn>2</mml:mn></mml:msub><mm Physical Review B, 2015, 92, .	1.1	37

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19	Independent particle theory with electron correlation. Journal of Chemical Physics, 2004, 120, 8395-8404.	1.2	35
20	Mercury Methylation by HgcA: Theory Supports Carbanion Transfer to Hg(II). Inorganic Chemistry, 2014, 53, 772-777.	1.9	34
21	Computational Investigation of the Pyrolysis Product Selectivity for Î±-Hydroxy Phenethyl Phenyl Ether and Phenethyl Phenyl Ether: Analysis of Substituent Effects and Reactant Conformer Selection. Journal of Physical Chemistry A, 2013, 117, 3235-3242.	1.1	33
22	Fast MAS ¹H NMR Study of Water Adsorption and Dissociation on the (100) Surface of Ceria Nanocubes: A Fully Hydroxylated, Hydrophobic Ceria Surface. Journal of Physical Chemistry C, 2017, 121, 7450-7465.	1.5	26
23	Below-Room-Temperature Câ€“H Bond Breaking on an Inexpensive Metal Oxide: Methanol to Formaldehyde on CeO₂(111). Journal of Physical Chemistry Letters, 2017, 8, 5810-5814.	2.1	24
24	Insights into amine-based CO2 capture: an ab initio self-consistent reaction field investigation. Structural Chemistry, 2011, 22, 537-549.	1.0	21
25	Charge decomposition analysis of the chemisorption bond. Chemical Physics Letters, 2000, 320, 222-228.	1.2	20
26	Ensuring N-representability: Coleman's algorithm. Chemical Physics Letters, 2002, 355, 263-269.	1.2	18
27	Correlated one-particle method: Numerical results. Journal of Chemical Physics, 2005, 123, 154103.	1.2	17
28	One-dimensional anharmonic oscillator: Quantum versus classical vibrational partition functions. Chemical Physics Letters, 2010, 493, 200-205.	1.2	16
29	CO2 capture in aqueous ammonia solutions: a computational chemistry perspective. Physical Chemistry Chemical Physics, 2012, 14, 16301.	1.3	15
30	Direct Î”MBPT(2) method for ionization potentials, electron affinities, and excitation energies using fractional occupation numbers. Journal of Chemical Physics, 2013, 138, 074101.	1.2	15
31	Coadsorbed Species Explain the Mechanism of Methanol Temperature-Programmed Desorption on CeO₂(111). Journal of Physical Chemistry C, 2016, 120, 7241-7247.	1.5	14
32	Hydrogen and methoxy coadsorption in the computation of the catalytic conversion of methanol on the ceria (111) surface. Surface Science, 2016, 648, 242-249.	0.8	9
33	Dehydrogenation of methanol to formaldehyde catalyzed by pristine and defective ceria surfaces. Physical Chemistry Chemical Physics, 2016, 18, 9990-9998.	1.3	9
34	The electronic structure of SiO3: a problematic example for coupled cluster methods. Chemical Physics Letters, 2002, 366, 100-108.	1.2	8
35	Ab initio study of hydrogen abstraction reactions on toluene and tetralin. Computational and Theoretical Chemistry, 2008, 851, 232-241.	1.5	8
36	Charge state switching of the divacancy defect in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>4</mml:mn><mml:mi>H</mml:mi></mml:math> -SiC. Physical Review B, 2018, 98, .	1.1	7

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37	Mechanisms of acetylcholinesterase protection against sarin and soman by adenosine A1 receptor agonist N6-cyclopentyladenosine. Computational Biology and Chemistry, 2018, 75, 74-81.	1.1	7
38	Multiresolution computational chemistry. Journal of Physics: Conference Series, 2005, 16, 243-246.	0.3	6
39	Electron transport in open systems from finite-size calculations: Examination of the principal layer method applied to linear gold chains. Journal of Chemical Physics, 2008, 128, 154713.	1.2	4
40	Methyl Formate Formation during Methanol Conversion over the (111) Ceria Surface. Journal of Physical Chemistry C, 2017, 121, 9920-9928.	1.5	4
41	Methanol adsorption and dissociation on LaMnO3 and Sr doped LaMnO3 (001) surfaces. Surface Science, 2017, 664, 155-161.	0.8	4
42	Advancing Understanding and Design of Functional Materials Through Theoretical and Computational Chemical Physics. , 2012, , 209-278.		3
43	Molecular Inclusion of Small Aging Products into the Hexanitrohexaazaisowurtzitane (CLâ€20) Lattice: Part I, Infrared Spectra. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.0	2
44	Molecular Inclusion of Small Aging Products into the Hexanitrohexaazaisowurtzitane (CLâ€20) Lattice: Part II, Polymorph Dependence. Propellants, Explosives, Pyrotechnics, 0, , .	1.0	1