# Ariana Beste

List of Publications by Year
in descending order

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Version: 2024-02-01

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

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Molecular Inclusion of Small Aging Products into the Hexanitrohexaazaisowurtzitane (CLâ€20) Lattice: Part I, Infrared Spectra. Propellants, Explosives, Pyrotechnics, 2022, 47, . | 1.0 | 2 |
| 2 | 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 |
| 3 | 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 |
| 4 | Methyl Formate Formation during Methanol Conversion over the (111) Ceria Surface. Journal of Physical Chemistry C, 2017, 121, 9920-9928. | 1.5 | 4 |
| 5 | Methanol adsorption and dissociation on LaMnO3 and Sr doped LaMnO3 (001) surfaces. Surface Science, 2017, 664, 155-161. | 0.8 | 4 |
| 6 | Fast MAS <sup>1</sup>H 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 |
| 7 | Below-Room-Temperature Câ€“H Bond Breaking on an Inexpensive Metal Oxide: Methanol to Formaldehyde on CeO<sub>2</sub>(111). Journal of Physical Chemistry Letters, 2017, 8, 5810-5814. | 2.1 | 24 |
| 8 | 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 |
| 9 | Coadsorbed Species Explain the Mechanism of Methanol Temperature-Programmed Desorption on CeO<sub>2</sub>(111). Journal of Physical Chemistry C, 2016, 120, 7241-7247. | 1.5 | 14 |
| 10 | 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 |
| 11 | Dehydrogenation of methanol to formaldehyde catalyzed by pristine and defective ceria surfaces. Physical Chemistry Chemical Physics, 2016, 18, 9990-9998. | 1.3 | 9 |
| 12 | 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 |
| 13 | 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 |
| 14 | ReaxFF Study of the Oxidation of Softwood Lignin in View of Carbon Fiber Production. Energy & Fuels, 2014, 28, 7007-7013. | 2.5 | 37 |
| 15 | Density Functional Theory Study of the Concerted Pyrolysis Mechanism for Lignin Models. Energy & Fuels, 2014, 28, 5229-5235. | 2.5 | 80 |
| 16 | Mercury Methylation by HgcA: Theory Supports Carbanion Transfer to Hg(II). Inorganic Chemistry, 2014, 53, 772-777. | 1.9 | 34 |
| 17 | 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 |
| 18 | Pyrolysis Pathways of Sulfonated Polyethylene, an Alternative Carbon Fiber Precursor. Journal of the American Chemical Society, 2013, 135, 6130-6141. | 6.6 | 60 |

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|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Computational study of bond dissociation enthalpies for lignin model compounds: Î²-5 Arylcoumaran. Chemical Physics Letters, 2012, 545, 100-106. | 1.2 | 73 |
| 22 | 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 |
| 23 | CO2 capture in aqueous ammonia solutions: a computational chemistry perspective. Physical Chemistry Chemical Physics, 2012, 14, 16301. | 1.3 | 15 |
| 24 | 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 |
| 25 | Advancing Understanding and Design of Functional Materials Through Theoretical and Computational Chemical Physics. , 2012, , 209-278. | | 3 |
| 26 | 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 |
| 27 | Insights into amine-based CO2 capture: an ab initio self-consistent reaction field investigation. Structural Chemistry, 2011, 22, 537-549. | 1.0 | 21 |
| 28 | Computational Study of Bond Dissociation Enthalpies for Substituted Î²â€Oâ€4 Lignin Model Compounds. ChemPhysChem, 2011, 12, 3556-3565. | 1.0 | 91 |
| 29 | One-dimensional anharmonic oscillator: Quantum versus classical vibrational partition functions. Chemical Physics Letters, 2010, 493, 200-205. | 1.2 | 16 |
| 30 | 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 |
| 31 | 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 |
| 32 | 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 |
| 33 | Ab initio study of hydrogen abstraction reactions on toluene and tetralin. Computational and Theoretical Chemistry, 2008, 851, 232-241. | 1.5 | 8 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Multiresolution computational chemistry. Journal of Physics: Conference Series, 2005, 16, 243-246. | 0.3 | 6 |
| 38 | Correlated one-particle method: Numerical results. Journal of Chemical Physics, 2005, 123, 154103. | 1.2 | 17 |
| 39 | Independent particle theory with electron correlation. Journal of Chemical Physics, 2004, 120, 8395-8404. | 1.2 | 35 |
| 40 | Ensuring N-representability: Coleman's algorithm. Chemical Physics Letters, 2002, 355, 263-269. | 1.2 | 18 |
| 41 | The electronic structure of SiO3: a problematic example for coupled cluster methods. Chemical Physics Letters, 2002, 366, 100-108. | 1.2 | 8 |
| 42 | Charge decomposition analysis of the chemisorption bond. Chemical Physics Letters, 2000, 320, 222-228. | 1.2 | 20 |
| 43 | 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 |
| 44 | Molecular Inclusion of Small Aging Products into the Hexanitrohexaazaisowurtzitane (CLâ€20) Lattice: Part II, Polymorph Dependence. Propellants, Explosives, Pyrotechnics, 0, , . | 1.0 | 1 |