Julianna Olah

List of Publications by Year
in descending order

59 papers	1,369 citations	489802 18 h-index	388640 36 g-index
60 all docs	60 docs citations	60 times ranked	1721 citing authors

#	Article	IF	Citations
1	Active site dynamics and catalytic mechanism in arabinan hydrolysis catalyzed by GH43 endo-arabinanase from QM/MM molecular dynamics simulation and potential energy surface. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7439-7449.	2.0	7
2	The Structure-Derived Mechanism of Box H/ACA Pseudouridine Synthase Offers a Plausible Paradigm for Programmable RNA Editing. ACS Catalysis, 2022, 12, 2756-2769.	5.5	5
3	Role of water coordination at zinc binding site and its catalytic pathway of dizinc creatininase: insights from quantum cluster approach. Journal of Computer-Aided Molecular Design, 2022, 36, 279-289.	1.3	5
4	H₂ and N₂ Binding Affinities Are Coupled in Synthetic Fe Nitrogenases Limiting N₂ Fixation. Organometallics, 2022, 41, 1134-1146.	1.1	3
5	Theoretical insights into water network of B-DNA duplex with Watson-Crick and Hoogsteen base pairing geometries. Journal of Molecular Liquids, 2022, 362, 119728.	2.3	1
6	Iron(<scp>ii</scp>) pillared-layer responsive frameworks via â€œkagomÃ© dualâ€•(kgd) supramolecular tessellations. Inorganic Chemistry Frontiers, 2021, 8, 3532-3546.	3.0	8
7	The Reactivity of Human and Equine Estrogen Quinones towards Purine Nucleosides. Symmetry, 2021, 13, 1641.	1.1	0
8	DFT study of formation and properties of dinuclear zirconocene cations: Effects of ligand structure, solvent, and metal on the dimerization process. Journal of Organometallic Chemistry, 2020, 905, 121024.	0.8	6
9	Demonstrating the Direct Relationship between Hydrogen Evolution Reaction and Catalyst Deactivation in Synthetic Fe Nitrogenases. ACS Catalysis, 2020, 10, 12555-12568.	5.5	13
10	Online conferences â€“ Towards a new (virtual) reality. Computational and Theoretical Chemistry, 2020, 1189, 112975.	1.1	42
11	Gas Sensing by Bacterial H-NOX Proteins: An MD Study. Molecules, 2020, 25, 2882.	1.7	6
12	Exploring Hydrogen Evolution Accompanying Nitrogen Reduction on Biomimetic Nitrogenase Analogs: Can Feâ€“NxHyIntermediates Be Active Under Turnover Conditions?. Inorganic Chemistry, 2019, 58, 7969-7977.	1.9	8
13	First Principles Calculation of the Reaction Rates for Ligand Binding to Myoglobin: The Cases of NO and CO. Chemistry - A European Journal, 2018, 24, 5350-5358.	1.7	6
14	Quantum chemical calculations support pseudouridine synthase reaction through a glycal intermediate and provide details of the mechanism. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	5
15	Identifying the Rate-Limiting Elementary Steps of Nitrogen Fixation with Single-Site Fe Model Complexes. Inorganic Chemistry, 2018, 57, 8499-8508.	1.9	19
16	Spin Crossover Behavior in a Homologous Series of Iron(II) Complexes Based on Functionalized Bipyridyl Ligands. Inorganic Chemistry, 2018, 57, 9880-9891.	1.9	36
17	Water-formamide mixtures: Topology of the hydrogen-bonded network. Journal of Molecular Liquids, 2017, 228, 25-31.	2.3	20
18	Combined Docking and Quantum Chemical Study on CYP-Mediated Metabolism of Estrogens in Man. Chemical Research in Toxicology, 2017, 30, 583-594.	1.7	5

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19	Hydration sphere structure of proteins: A theoretical study. Journal of Molecular Liquids, 2017, 238, 462-469.	2.3	12
20	How can we detect hydrogen bond local cooperativity in liquid water: A simulation study. Journal of Molecular Liquids, 2017, 245, 140-146.	2.3	13
21	Dual Role of the Active Site Residues of Thermus thermophilus 3-Isopropylmalate Dehydrogenase: Chemical Catalysis and Domain Closure. Biochemistry, 2016, 55, 560-574.	1.2	2
22	Synthesis, experimental and theoretical studies on the factors influencing the pKa values of new crown ethers containing a diarylphosphinic acid unit. Tetrahedron, 2016, 72, 8593-8602.	1.0	2
23	Accurate modeling of cationâ€“Ï€ interactions in enzymes: a case study on the CDPCho:phosphocholine cytidylyltransferase complex. Structural Chemistry, 2015, 26, 1411-1423.	1.0	3
24	Glutamate 270 plays an essential role in K⁺â€activation and domain closure of Thermus thermophilus isopropylmalate dehydrogenase. FEBS Letters, 2015, 589, 240-245.	1.3	5
25	Convergence of Atomic Charges with the Size of the Enzymatic Environment. Journal of Chemical Information and Modeling, 2015, 55, 564-571.	2.5	17
26	How does the protein environment optimize the thermodynamics of thiol sulfenylation? Insights from model systems to QM/MM calculations on human 2-Cys peroxiredoxin. Journal of Biomolecular Structure and Dynamics, 2015, 33, 584-596.	2.0	8
27	The mechanism of human aromatase (CYP 19A1) revisited: DFT and QM/MM calculations support a compound I-mediated pathway for the aromatization process. Structural Chemistry, 2015, 26, 279-300.	1.0	12
28	Molecular Mechanism for the Thermo-Sensitive Phenotype of CHO-MT58 Cell Line Harbouring a Mutant CTP:Phosphocholine Cytidylyltransferase. PLoS ONE, 2015, 10, e0129632.	1.1	10
29	Structural and energetic basis of isopropylmalate dehydrogenase enzyme catalysis. FEBS Journal, 2014, 281, 5063-5076.	2.2	16
30	Enolization as an Alternative Proton Delivery Pathway in Human Aromatase (P450 19A1). Journal of Physical Chemistry B, 2014, 118, 390-405.	1.2	14
31	Hydrogen bond network topology in liquid water and methanol: a graph theory approach. Physical Chemistry Chemical Physics, 2013, 15, 15163.	1.3	60
32	Evolutionary and mechanistic insights into substrate and product accommodation of <scp>CTP</scp>:phosphocholine cytidylyltransferase from <scp>P</scp>lasmodiumÂfalciparum. FEBS Journal, 2013, 280, 3132-3148.	2.2	16
33	Oxazol-2-ylidenes. A new class of stable carbenes?. RSC Advances, 2013, 3, 7970.	1.7	32
34	Quantum Mechanical Modeling: A Tool for the Understanding of Enzyme Reactions. Biomolecules, 2013, 3, 662-702.	1.8	21
35	Direct Hydride Shift Mechanism and Stereoselectivity of P450_{nor} Confirmed by QM/MM Calculations. Journal of Physical Chemistry B, 2012, 116, 872-885.	1.2	23
36	Solution behavior of iron(<scp>iii</scp>) and iron(<scp>ii</scp>) porphyrins in DMSO and reaction with superoxide. Effect of neighboring positive charge on thermodynamics, kinetics and nature of iron-(su)peroxo product. Dalton Transactions, 2012, 41, 546-557.	1.6	18

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37	Does Compound I Vary Significantly between Isoforms of Cytochrome P450?. Journal of the American Chemical Society, 2011, 133, 15464-15474.	6.6	188
38	Understanding the determinants of selectivity in drug metabolism through modeling of dextromethorphan oxidation by cytochrome P450. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6050-6055.	3.3	98
39	Studies on an iron(iii)-peroxo porphyrin. Iron(iii)-peroxo or iron(ii)-superoxo?. Dalton Transactions, 2010, 39, 2049.	1.6	33
40	Combining the chemistries of silylene and sulfur-nitrogen compoundsâ€"SiS2N2 and related systems. Dalton Transactions, 2010, 39, 3256.	1.6	4
41	Nucleophilicity and electrophilicity of silylenes from a molecular electrostatic potential and dual descriptor perspectives. Chemical Physics Letters, 2009, 470, 180-186.	1.2	17
42	NO Bonding to Heme Groups: DFT and Correlated ab Initio Calculations. Journal of Physical Chemistry A, 2009, 113, 7338-7345.	1.1	84
43	Synthesis of vinca alkaloids and related compounds. Part 110: A new synthetic method for the preparation of pandoline-type alkaloid-like molecules. Tetrahedron, 2008, 64, 7949-7955.	1.0	4
44	Mechanism of Water Addition to Silatriafulvenes and Silapentafulvenes. Organometallics, 2008, 27, 2723-2729.	1.1	7
45	Silylenes:Â A Unified Picture of Their Stability, Acidâ^'Base and Spin Properties, Nucleophilicity, and Electrophilicity via Computational and Conceptual Density Functional Theory. Journal of Physical Chemistry A, 2007, 111, 10815-10823.	1.1	40
46	Relationship between electrophilicity and spin-philicity of divalent and monovalent species of group 14 and 15 elements. Computational and Theoretical Chemistry, 2006, 771, 135-140.	1.5	8
47	On the Usefulness of Bond Orders and Overlap Populations to Chalcogen-Nitrogen Systems. European Journal of Inorganic Chemistry, 2006, 2006, 69-77.	1.0	17
48	Spin-philicity and spin-donicity of simple nitrenes and phosphinidenes. Chemical Physics Letters, 2005, 401, 337-341.	1.2	29
49	Is there a satisfactory description of the molecular structure of Roeskyâ€™s ketone?. Chemical Physics Letters, 2005, 413, 440-444.	1.2	11
50	Drude-type conductivity of charged sphere colloidal crystals: Density and temperature dependence. Journal of Chemical Physics, 2005, 123, 104903.	1.2	24
51	Hardâ^'Soft Acidâ^'Base Interactions of Silylenes and Germylenes. Journal of Physical Chemistry A, 2005, 109, 1608-1615.	1.1	66
52	NaSCN: Striking Differences Between Its Gas-Phase and Crystal-Phase Structure: A Theoretical Study. ChemInform, 2004, 35, no.	0.1	0
53	Spin-Philicity and Spin-Donicity of Substituted Carbenes, Silylenes, Germylenes, and Stannylenes. Journal of Physical Chemistry A, 2004, 108, 490-499.	1.1	60
54	NaSCN:Â Striking Differences between Its Gas-Phase and Crystal-Phase Structure: A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 8400-8406.	1.1	9

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55	Relationship between stability and dimerization ability of silylenes. Journal of Organometallic Chemistry, 2003, 686, 112-117.	0.8	21
56	Molecular structure and internal rotation potential of perfluoro (2,4-dimethyl-3-oxa-2,4-diazapentane), (CF3)2Nâ€“Oâ€“N(CF3)2. Computational and Theoretical Chemistry, 2003, 620, 157-163.	1.5	0
57	Condensed Fukui Functions Derived from Stockholder Charges:â€‰ Assessment of Their Performance as Local Reactivity Descriptors. Journal of Physical Chemistry A, 2002, 106, 3885-3890.	1.1	168
58	Organizing atomic partial charges into a database. Computational and Theoretical Chemistry, 2002, 589-590, 1-5.	1.5	1
59	The mechanism of biochemical NOâ€sensing: insights from computational chemistry. Chemistry - A European Journal, 0, , .	1.7	1