Hui-Hsu Gavin Tsai

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	TD-DFT Study of the Excited-State Potential Energy Surfaces of 2-(2′-Hydroxyphenyl)benzimidazole and its Amino Derivatives. Journal of Physical Chemistry A, 2010, 114, 4065-4079.	2.5	85
2	Coupling Molecular Dynamics Simulations with Experiments for the Rational Design of Indolicidin-Analogous Antimicrobial Peptides. Journal of Molecular Biology, 2009, 392, 837-854.	4.2	52
3	Sequence and Structure Analysis of Parallel β Helices: Implication for Constructing Amyloid Structural Models. Structure, 2006, 14, 1059-1072.	3.3	40
4	Effects of Internal Electron-Withdrawing Moieties in D–Aâ^'π–A Organic Sensitizers on Photophysical Properties for DSSCs: A Computational Study. ACS Omega, 2018, 3, 433-445.	3.5	35
5	Molecular dynamics simulation of cation–phospholipid clustering in phospholipid bilayers: Possible role in stalk formation during membrane fusion. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 2742-2755.	2.6	33
6	Asymmetric Synthesis of (–)‣entiginosine by Double Azaâ€Michael Reaction. European Journal of Organic Chemistry, 2010, 2010, 4771-4773.	2.4	29
7	Organocatalyzed Enantioselective Michael Addition of 2â€Hydroxypyridines and α,βâ€Unsaturated 1,4â€Dicarbonyl Compounds. Advanced Synthesis and Catalysis, 2019, 361, 4966-4982.	4.3	26
8	Folding and membrane insertion of amyloidâ€beta (25–35) peptide and its mutants: Implications for aggregation and neurotoxicity. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1909-1925.	2.6	25
9	Probing the Nature and Local Structure of Phosphonic Acid Groups Functionalized in Mesoporous Silica SBA-15. Journal of Physical Chemistry C, 2012, 116, 1658-1669.	3.1	25
10	Direct Evidence for Interactions between Acidic Functional Groups and Silanols in Cubic Mesoporous Organosilicas. Journal of the American Chemical Society, 2008, 130, 11566-11567.	13.7	24
11	Location and Conformation of Amyloid β(25–35) Peptide and its Sequenceâ€Shuffled Peptides within Membranes: Implications for Aggregation and Toxicity in PC12 Cells. ChemMedChem, 2014, 9, 1002-1011.	3.2	19
12	Long-Range Olefin Isomerization Catalyzed by Palladium(0) Nanoparticles. ACS Omega, 2017, 2, 698-711.	3.5	18
13	Ligand Exchange in the Synthesis of Metal–Organic Frameworks Occurs Through Acid-Catalyzed Associative Substitution. Inorganic Chemistry, 2019, 58, 14457-14466.	4.0	18
14	Fluoreneâ€Containing Organic Photosensitizers for Dyeâ€Sensitized Solar Cells. ChemPlusChem, 2012, 77, 832-843.	2.8	17
15	Multi-step formation of a hemifusion diaphragm for vesicle fusion revealed by all-atom molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1529-1535.	2.6	17
16	Geometrical effects of phospholipid olefinic bonds on the structure and dynamics of membranes: A molecular dynamics study. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1234-1247.	2.6	17
17	Osmium sensitizer with enhanced spin–orbit coupling for panchromatic dye-sensitized solar cells. Journal of Materials Chemistry A, 2020, 8, 12361-12369.	10.3	17
18	Synthesis and solid-state NMR characterization of cubic mesoporous silica SBA-1 functionalized with sulfonic acid groups. Journal of Colloid and Interface Science, 2011, 359, 86-94.	9.4	15

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19	Oxidative transformation of thiol groups to disulfide bonds in mesoporous silicas: a diagnostic reaction for probing distribution of organic functional groups. New Journal of Chemistry, 2009, 33, 2199.	2.8	11
20	A Molecular Dynamics Study of the Structural and Dynamical Properties of Putative Arsenic Substituted Lipid Bilayers. International Journal of Molecular Sciences, 2013, 14, 7702-7715.	4.1	10
21	Molecular mechanism of Ca2+-catalyzed fusion of phospholipid micelles. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 2729-2738.	2.6	7
22	Interplay of Hydrogenation and Dehydrogenation in Isoindoline and Indoline Isomers: A Density Functional Theory Study. Journal of Physical Chemistry A, 2008, 112, 5278-5285.	2.5	5
23	First-Principles Investigation of the Thermal Degradation Mechanisms of Methylammonium Lead Triiodide Perovskite. Journal of Physical Chemistry C, 2020, 124, 14521-14530.	3.1	5
24	The Arginine Pairs and C-Termini of the Sso7c4 from Sulfolobus solfataricus Participate in Binding and Bending DNA. PLoS ONE, 2017, 12, e0169627.	2.5	4
25	Unusually Longâ€Wavelength Emissions of Cyclopropanes: New Insight into Câ^'C Bond Homolysis. Chemistry - A European Journal, 2018, 24, 7595-7600.	3.3	4
26	Terpyridyl Ruthenium Complexes Functionalized with Conjugated Heterocycles for Panchromatic Dye-Sensitized Solar Cells. ACS Applied Energy Materials, 2021, 4, 13461-13470.	5.1	3
27	Double Proton Transfer during a Novel Tertiary α-Ketol Rearrangement in Ketol-Acid Reductoisomerase: A Water-Mediated, Metal-Catalyzed, Base-Induced Mechanism. Journal of Physical Chemistry B, 2021, 125, 11893-11906.	2.6	2