## Hui-Hsu Gavin Tsai

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	Terpyridyl Ruthenium Complexes Functionalized with Conjugated Heterocycles for Panchromatic Dye-Sensitized Solar Cells. ACS Applied Energy Materials, 2021, 4, 13461-13470.	5.1	3
3	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
4	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
5	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
6	Ligand Exchange in the Synthesis of Metal–Organic Frameworks Occurs Through Acid-Catalyzed Associative Substitution. Inorganic Chemistry, 2019, 58, 14457-14466.	4.0	18
7	Unusually Longâ€Wavelength Emissions of Cyclopropanes: New Insight into Câ^C Bond Homolysis. Chemistry - A European Journal, 2018, 24, 7595-7600.	3.3	4
8	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
9	Long-Range Olefin Isomerization Catalyzed by Palladium(0) Nanoparticles. ACS Omega, 2017, 2, 698-711.	3.5	18
10	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
11	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
12	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
13	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
14	Molecular mechanism of Ca2+-catalyzed fusion of phospholipid micelles. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 2729-2738.	2.6	7
15	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
16	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
17	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
18	Fluoreneâ€Containing Organic Photosensitizers for Dyeâ€5ensitized Solar Cells. ChemPlusChem, 2012, 77, 832-843.	2.8	17

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19	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
20	Asymmetric Synthesis of (–)‣entiginosine by Double Azaâ€Michael Reaction. European Journal of Organic Chemistry, 2010, 2010, 4771-4773.	2.4	29
21	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
22	TD-DFT Study of the Excited-State Potential Energy Surfaces of 2-(2â€2-Hydroxyphenyl)benzimidazole and its Amino Derivatives. Journal of Physical Chemistry A, 2010, 114, 4065-4079.	2.5	85
23	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
24	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
25	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
26	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
27	Sequence and Structure Analysis of Parallel Î <sup>2</sup> Helices: Implication for Constructing Amyloid Structural Models. Structure, 2006, 14, 1059-1072.	3.3	40