

Annapaola Migani

List of Publications by Year in descending order

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49
papers

3,186
citations

168829

31
h-index

214428

50
g-index

51
all docs

51
docs citations

51
times ranked

4683
citing authors

#	ARTICLE	IF	CITATIONS
1	Phosphorus-Doped Graphene as a Metal-Free Material for Thermochemical Water Reforming at Unusually Mild Conditions. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 838-846.	3.2	28
2	Theoretical study of non-Hammett <i>vs.</i> Hammett behaviour in the thermolysis and photolysis of arylchlorodiazirines. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1181-1188.	1.3	15
3	What Controls Photocatalytic Water Oxidation on Rutile TiO ₂ (110) under Ultra-High-Vacuum Conditions?. <i>Journal of the American Chemical Society</i> , 2017, 139, 11845-11856.	6.6	48
4	Optical Absorption Spectra and Excitons of Dye-Substrate Interfaces: Catechol on TiO ₂ (110). <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2843-2852.	2.3	31
5	Excitonic Interfacial Proton-Coupled Electron Transfer Mechanism in the Photocatalytic Oxidation of Methanol to Formaldehyde on TiO ₂ (110). <i>Journal of the American Chemical Society</i> , 2016, 138, 16165-16173.	6.6	64
6	Early events in the photochemistry of 5-diazo Meldrum's acid: formation of a product manifold in Câ€“N bound and pre-dissociated intersection seam regions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30785-30793.	1.3	11
7	Quasiparticle Interfacial Level Alignment of Highly Hybridized Frontier Levels: H ₂ O on TiO ₂ (110). <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 239-251.	2.3	28
8	Using <i>G₀W₀</i> Level Alignment to Identify Catechol's Structure on TiO ₂ (110). <i>Journal of Physical Chemistry C</i> , 2015, 119, 19634-19641.	1.5	13
9	Comparing Quasiparticle H ₂ O Level Alignment on Anatase and Rutile TiO ₂ . <i>ACS Catalysis</i> , 2015, 5, 4242-4254.	5.5	50
10	Coverage dependence of the level alignment for methanol on TiO ₂ (110). <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 259-265.	1.1	13
11	Oxygen vacancies in self-assemblies of ceria nanoparticles. <i>Journal of Materials Chemistry A</i> , 2014, 2, 18329-18338.	5.2	33
12	Quasiparticle Level Alignment for Photocatalytic Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2103-2113.	2.3	60
13	Level Alignment of a Prototypical Photocatalytic System: Methanol on TiO ₂ (110). <i>Journal of the American Chemical Society</i> , 2013, 135, 11429-11432.	6.6	68
14	Gold and Methane: A Noble Combination for Delicate Oxidation. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3006-3012.	2.1	28
15	Irreversible phototautomerization of o-phthalaldehyde through electronic relocation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6561.	1.3	19
16	Octahedrality versus tetrahedrality in stoichiometric ceria nanoparticles. <i>Chemical Communications</i> , 2012, 48, 4199.	2.2	25
17	Wave Packet Dynamics at an Extended Seam of Conical Intersection: Mechanism of the Light-Induced Wolff Rearrangement. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1056-1061.	2.1	32
18	Effects of deposited Pt particles on the reducibility of CeO ₂ (111). <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11384.	1.3	89

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19	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. <i>Chemical Communications</i> , 2011, 47, 6383.	2.2	33
20	A non-adiabatic quantum-classical dynamics study of the intramolecular excited state hydrogen transfer in ortho-nitrobenzaldehyde. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14685.	1.3	17
21	Formation of Superoxide Anions on Ceria Nanoparticles by Interaction of Molecular Oxygen with Ce ³⁺ Sites. <i>Journal of Physical Chemistry C</i> , 2011, 115, 5817-5822.	1.5	107
22	Density Functional Modeling of the Interactions of Platinum Clusters with CeO ₂ Nanoparticles of Different Size. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16081-16086.	1.5	40
23	Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. <i>Nature Materials</i> , 2011, 10, 310-315.	13.3	748
24	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. <i>Chemical Communications</i> , 2010, 46, 5936.	2.2	160
25	A global picture of the S ₁ /S ₀ conical intersection seam of benzene. <i>Chemical Physics</i> , 2010, 377, 60-65.	0.9	61
26	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. <i>Journal of Materials Chemistry</i> , 2010, 20, 10535.	6.7	192
27	Exploring Ce ³⁺ /Ce ⁴⁺ cation ordering in reduced ceria nanoparticles using interionic-potential and density-functional calculations. <i>Journal of Chemical Physics</i> , 2009, 131, 064701.	1.2	50
28	MS-CASPT2 Assignment of the UV/Vis Absorption Spectrum of Diazoquinones Undergoing the Photoinduced Wolff Rearrangement. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9413-9417.	1.1	13
29	Benign Decay vs. Photolysis in the Photophysics and Photochemistry of 5-Bromouracil. A Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5489-5495.	1.1	19
30	Towards size-converged properties of model ceria nanoparticles: Monitoring by adsorbed CO using DFT +U approach. <i>Chemical Physics Letters</i> , 2008, 465, 106-109.	1.2	31
31	Density functional studies of model cerium oxide nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5730.	1.3	125
32	Electronic States of <i>o</i> -Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5046-5053.	1.1	30
33	An Extended Conical Intersection Seam Associated with a Manifold of Decay Paths: Excited-State Intramolecular Proton Transfer in <i>O</i> -Hydroxybenzaldehyde. <i>Journal of the American Chemical Society</i> , 2008, 130, 6932-6933.	6.6	64
34	Modeling Thymine Photodimerizations in DNA: Mechanism and Correlation Diagrams. <i>Journal of the American Chemical Society</i> , 2007, 129, 14540-14541.	6.6	88
35	Photostability versus Photodegradation in the Excited-State Intramolecular Proton Transfer of Nitro Enamines: A Competing Reaction Paths and Conical Intersections. <i>Journal of the American Chemical Society</i> , 2007, 129, 3703-3713.	6.6	32
36	Benign and Degrading Excited-State Processes of DNA Nucleobases and their Derivatives. <i>AIP Conference Proceedings</i> , 2007, , .	0.3	0

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37	Water effect on the excited-state decay paths of singlet excited cytosine. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007, 190, 283-289.	2.0	43
38	Requirements for the generalization of the ab initio two-state model for external electric field induced electron transfer at electrodes. <i>Journal of Electroanalytical Chemistry</i> , 2007, 607, 25-36.	1.9	1
39	A Systematic Study of the Structure and Bonding of Halogens on Low-Index Transition Metal Surfaces. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11894-11906.	1.2	93
40	Chemisorption of atomic chlorine on metal surfaces and the interpretation of the induced work function changes. <i>Surface Science</i> , 2005, 574, 297-305.	0.8	66
41	Electric field induced electron transfer at the adsorbate-surface interface. Effect of the type of metal surface. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3353.	1.3	6
42	The Ring-Opening Reaction of Chromenes: A Photochemical Mode-Dependent Transformation. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8684-8692.	1.1	41
43	CONICAL INTERSECTIONS AND ORGANIC REACTION MECHANISMS. <i>Advanced Series in Physical Chemistry</i> , 2004, , 271-320.	1.5	50
44	Structure of the intersection space associated with Z/E photoisomerization of retinal in rhodopsin proteins. <i>Faraday Discussions</i> , 2004, 127, 179-191.	1.6	60
45	Probing the Photochemical Funnel of a Retinal Chromophore Model via Zero-Point Energy Sampling Semiclassical Dynamics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4685-4693.	1.1	81
46	CASPT2//CASSCF and TDDFT//CASSCF Mapping of the Excited State Isomerization Path of a Minimal Model of the Retinal Chromophore. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1208-1213.	1.1	82
47	Design and Photochemical Characterization of a Biomimetic Light-Driven Z/E Switcher. <i>Journal of the American Chemical Society</i> , 2004, 126, 9349-9359.	6.6	58
48	Relationship between Photoisomerization Path and Intersection Space in a Retinal Chromophore Model. <i>Journal of the American Chemical Society</i> , 2003, 125, 2804-2808.	6.6	110
49	Photoisomerization acceleration in retinal protonated Schiff-base models. <i>Photochemical and Photobiological Sciences</i> , 2003, 2, 1250.	1.6	25