Annapaola Migani

List of Publications by Year
in descending order

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49 papers	3,186 citations	147801 31 h-index	189892 50 g-index
51 all docs	51 docs citations	51 times ranked	4120 citing authors

#	Article	IF	Citations
1	Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. Nature Materials, 2011, 10, 310-315.	27.5	748
2	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. Journal of Materials Chemistry, 2010, 20, 10535.	6.7	192
3	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. Chemical Communications, 2010, 46, 5936.	4.1	160
4	Density functional studies of model cerium oxide nanoparticles. Physical Chemistry Chemical Physics, 2008, 10, 5730.	2.8	125
5	Relationship between Photoisomerization Path and Intersection Space in a Retinal Chromophore Model. Journal of the American Chemical Society, 2003, 125, 2804-2808.	13.7	110
6	Formation of Superoxide Anions on Ceria Nanoparticles by Interaction of Molecular Oxygen with Ce³⁺ Sites. Journal of Physical Chemistry C, 2011, 115, 5817-5822.	3.1	107
7	A Systematic Study of the Structure and Bonding of Halogens on Low-Index Transition Metal Surfaces. Journal of Physical Chemistry B, 2006, 110, 11894-11906.	2.6	93
8	Effects of deposited Pt particles on the reducibility of CeO2(111). Physical Chemistry Chemical Physics, 2011, 13, 11384.	2.8	89
9	Modeling Thymine Photodimerizations in DNA:â€‰ Mechanism and Correlation Diagrams. Journal of the American Chemical Society, 2007, 129, 14540-14541.	13.7	88
10	CASPT2//CASSCF and TDDFT//CASSCF Mapping of the Excited State Isomerization Path of a Minimal Model of the Retinal Chromophore. Journal of Physical Chemistry A, 2004, 108, 1208-1213.	2.5	82
11	Probing the Photochemical Funnel of a Retinal Chromophore Model via Zero-Point Energy Sampling Semiclassical Dynamics. Journal of Physical Chemistry A, 2004, 108, 4685-4693.	2.5	81
12	Level Alignment of a Prototypical Photocatalytic System: Methanol on TiO₂(110). Journal of the American Chemical Society, 2013, 135, 11429-11432.	13.7	68
13	Chemisorption of atomic chlorine on metal surfaces and the interpretation of the induced work function changes. Surface Science, 2005, 574, 297-305.	1.9	66
14	An Extended Conical Intersection Seam Associated with a Manifold of Decay Paths: Excited-State Intramolecular Proton Transfer in O-Hydroxybenzaldehyde. Journal of the American Chemical Society, 2008, 130, 6932-6933.	13.7	64
15	Excitonic Interfacial Proton-Coupled Electron Transfer Mechanism in the Photocatalytic Oxidation of Methanol to Formaldehyde on TiO₂(110). Journal of the American Chemical Society, 2016, 138, 16165-16173.	13.7	64
16	A global picture of the S1/S0 conical intersection seam of benzene. Chemical Physics, 2010, 377, 60-65.	1.9	61
17	Structure of the intersection space associated with Z/E photoisomerization of retinal in rhodopsin proteins. Faraday Discussions, 2004, 127, 179-191.	3.2	60
18	Quasiparticle Level Alignment for Photocatalytic Interfaces. Journal of Chemical Theory and Computation, 2014, 10, 2103-2113.	5.3	60

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19	Design and Photochemical Characterization of a Biomimetic Light-Driven Z/E Switcher. Journal of the American Chemical Society, 2004, 126, 9349-9359.	13.7	58
20	CONICAL INTERSECTIONS AND ORGANIC REACTION MECHANISMS. Advanced Series in Physical Chemistry, 2004, , 271-320.	1.5	50
21	Exploring Ce3+/Ce4+ cation ordering in reduced ceria nanoparticles using interionic-potential and density-functional calculations. Journal of Chemical Physics, 2009, 131, 064701.	3.0	50
22	Comparing Quasiparticle H₂O Level Alignment on Anatase and Rutile TiO₂. ACS Catalysis, 2015, 5, 4242-4254.	11.2	50
23	What Controls Photocatalytic Water Oxidation on Rutile TiO₂(110) under Ultra-High-Vacuum Conditions?. Journal of the American Chemical Society, 2017, 139, 11845-11856.	13.7	48
24	Water effect on the excited-state decay paths of singlet excited cytosine. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 283-289.	3.9	43
25	The Ring-Opening Reaction of Chromenes:Â A Photochemical Mode-Dependent Transformation. Journal of Physical Chemistry A, 2005, 109, 8684-8692.	2.5	41
26	Density Functional Modeling of the Interactions of Platinum Clusters with CeO₂ Nanoparticles of Different Size. Journal of Physical Chemistry C, 2011, 115, 16081-16086.	3.1	40
27	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. Chemical Communications, 2011, 47, 6383.	4.1	33
28	Oxygen vacancies in self-assemblies of ceria nanoparticles. Journal of Materials Chemistry A, 2014, 2, 18329-18338.	10.3	33
29	Photostability versus Photodegradation in the Excited-State Intramolecular Proton Transfer of Nitro Enamines:Â Competing Reaction Paths and Conical Intersections. Journal of the American Chemical Society, 2007, 129, 3703-3713.	13.7	32
30	Wave Packet Dynamics at an Extended Seam of Conical Intersection: Mechanism of the Light-Induced Wolff Rearrangement. Journal of Physical Chemistry Letters, 2012, 3, 1056-1061.	4.6	32
31	Towards size-converged properties of model ceria nanoparticles: Monitoring by adsorbed CO using DFT +U approach. Chemical Physics Letters, 2008, 465, 106-109.	2.6	31
32	Optical Absorption Spectra and Excitons of Dye-Substrate Interfaces: Catechol on TiO₂(110). Journal of Chemical Theory and Computation, 2016, 12, 2843-2852.	5.3	31
33	Electronic States of o-Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 5046-5053.	2.5	30
34	Gold and Methane: A Noble Combination for Delicate Oxidation. Journal of Physical Chemistry Letters, 2013, 4, 3006-3012.	4.6	28
35	Quasiparticle Interfacial Level Alignment of Highly Hybridized Frontier Levels: H₂O on TiO₂(110). Journal of Chemical Theory and Computation, 2015, 11, 239-251.	5.3	28
36	Phosphorus-Doped Graphene as a Metal-Free Material for Thermochemical Water Reforming at Unusually Mild Conditions. ACS Sustainable Chemistry and Engineering, 2019, 7, 838-846.	6.7	28

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37	Photoisomerization acceleration in retinal protonated Schiff-base models. Photochemical and Photobiological Sciences, 2003, 2, 1250.	2.9	25
38	Octahedrality versus tetrahedrality in stoichiometric ceria nanoparticles. Chemical Communications, 2012, 48, 4199.	4.1	25
39	Benign Decay vs. Photolysis in the Photophysics and Photochemistry of 5-Bromouracil. A Computational Study. Journal of Physical Chemistry A, 2009, 113, 5489-5495.	2.5	19
40	Irreversible phototautomerization of o-phthalaldehyde through electronic relocation. Physical Chemistry Chemical Physics, 2012, 14, 6561.	2.8	19
41	A non-adiabatic quantum-classical dynamics study of the intramolecular excited state hydrogen transfer in ortho-nitrobenzaldehyde. Physical Chemistry Chemical Physics, 2011, 13, 14685.	2.8	17
42	Theoretical study of non-Hammett vs. Hammett behaviour in the thermolysis and photolysis of arylchlorodiazirines. Physical Chemistry Chemical Physics, 2018, 20, 1181-1188.	2.8	15
43	MS-CASPT2 Assignment of the UV/Vis Absorption Spectrum of Diazoquinones Undergoing the Photoinduced Wolff Rearrangement. Journal of Physical Chemistry A, 2009, 113, 9413-9417.	2.5	13
44	Coverage dependence of the level alignment for methanol on TiO2(110). Computational and Theoretical Chemistry, 2014, 1040-1041, 259-265.	2.5	13
45	Using G₀W₀ Level Alignment to Identify Catecholâ€™s Structure on TiO₂(110). Journal of Physical Chemistry C, 2015, 119, 19634-19641.	3.1	13
46	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. Physical Chemistry Chemical Physics, 2016, 18, 30785-30793.	2.8	11
47	Electric field induced electron transfer at the adsorbateâ€“surface interface. Effect of the type of metal surface. Physical Chemistry Chemical Physics, 2005, 7, 3353.	2.8	6
48	Requirements for the generalization of the ab initio two-state model for external electric field induced electron transfer at electrodes. Journal of Electroanalytical Chemistry, 2007, 607, 25-36.	3.8	1
49	Benign and Degrading Excited-State Processes of DNA Nucleobases and their Derivatives. AIP Conference Proceedings, 2007, , .	0.4	0