Francesco Mercuri

List of Publications by Year
in descending order

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35 papers	749 citations	623734 14 h-index	526287 27 g-index
35 all docs	35 docs citations	35 times ranked	1100 citing authors

#	Article	IF	Citations
1	A Molecular Drone for Atomicâ€Scale Fabrication Working under Ambient Conditions. Advanced Materials, 2021, 33, e2007150.	21.0	5
2	Toward Real Setting Applications of Organic and Perovskite Solar Cells: A Comparative Review. Energy Technology, 2021, 9, 2000901.	3.8	33
3	Stiffness of Fluid and Gel Phase Lipid Nanovesicles: Weighting the Contributions of Membrane Bending Modulus and Luminal Pressurization. Langmuir, 2021, 37, 12027-12037.	3.5	10
4	Noncovalent passivation of supported phosphorene for device applications: from morphology to electronic properties. Physical Chemistry Chemical Physics, 2020, 22, 12482-12488.	2.8	6
5	3D versus 2D Electrolyteâ€“Semiconductor Interfaces in Rylenediimideâ€Based Electronâ€Transporting Waterâ€Gated Organic Fieldâ€Effect Transistors. Advanced Electronic Materials, 2020, 6, 2000638.	5.1	2
6	Efficient evaluation of Coulomb interactions in kinetic Monte Carlo simulations of charge transport. Journal of Chemical Physics, 2020, 152, 164102.	3.0	5
7	On the Nature of Charge-Injecting Contacts in Organic Field-Effect Transistors. ACS Applied Materials & Interfaces, 2020, 12, 30616-30626.	8.0	9
8	Epitaxial multilayers of alkanes on two-dimensional black phosphorus as passivating and electrically insulating nanostructures. Nanoscale, 2019, 11, 17252-17261.	5.6	13
9	A Computational Predictive Approach for Controlling the Morphology of Functional Molecular Aggregates on Substrates. Advanced Theory and Simulations, 2019, 2, 1900156.	2.8	7
10	Highâ€Performance and Stable Perovskite Solar Cells Based on Dopantâ€Free Arylamineâ€Substituted Copper(II) Phthalocyanine Holeâ€Transporting Materials. Advanced Energy Materials, 2019, 9, 1901019.	19.5	80
11	A Structural Model of a P450-Ferredoxin Complex from Orientation-Selective Double Electronâ€“Electron Resonance Spectroscopy. Journal of the American Chemical Society, 2018, 140, 2514-2527.	13.7	22
12	Nanoscale morphology and electronic coupling at the interface between indium tin oxide and organic molecular materials. Nanoscale, 2018, 10, 9376-9385.	5.6	14
13	Spatial and orientational dependence of electron transfer parameters in aggregates of iridium-containing host materials for OLEDs: coupling constrained density functional theory with molecular dynamics. Physical Chemistry Chemical Physics, 2018, 20, 28393-28399.	2.8	8
14	Synthesis and investigation on processing-depending polarized fluorescence emission in thin-films of 2,2â€²-([2,2â€²-bithiophene]-5,5â€²-diyl)bis(5-octyl-4-phenyl-4H-thieno[2,3-c]pyrrol-6(5H)-one). Journal of Materials Chemistry C, 2017, 5, 10320-10331.	5.5	5
15	Morphology and Electronic Properties of N,Nâ€²-Ditridecylperylene-3,4,9,10-tetracarboxylic Diimide Layered Aggregates: From Structural Predictions to Charge Transport. Journal of Physical Chemistry C, 2017, 121, 21857-21864.	3.1	14
16	A self-assembled lysinated perylene diimide film as a multifunctional material for neural interfacing. Journal of Materials Chemistry B, 2016, 4, 2921-2932.	5.8	8
17	Theoretical insights on morphology and charge transport properties of two-dimensional N,Nâ€²-ditridecylperylene-3,4,9,10-tetra carboxylic diimide aggregates. RSC Advances, 2016, 6, 40724-40730.	3.6	11
18	Correlation between gate-dielectric morphology at the nanoscale and charge transport properties in organic field-effect transistors. RSC Advances, 2015, 5, 11797-11805.	3.6	15

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19	Evidence of benzenoid domains in nanographenes. Physical Chemistry Chemical Physics, 2015, 17, 2088-2093.	2.8	6
20	Correlation between atomistic morphology and electron transport properties in defect-free and defected graphene nanoribbons: An interpretation through Clar sextet theory. Carbon, 2014, 75, 190-200.	10.3	6
21	Towards nano-organic chemistry: perspectives for a bottom-up approach to the synthesis of low-dimensional carbon nanostructures. Nanoscale, 2012, 4, 369-379.	5.6	27
22	Redox-switchable devices based on functionalized graphene nanoribbons. Nanoscale, 2012, 4, 1350.	5.6	12
23	Modeling of low-dimensional carbon nanostructures: an efficient approach based on chemical criteria. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, 2632-2635.	0.8	4
24	Atomistic engineering in the control of the electronic properties of CdSe nanotubes. Physical Review B, 2010, 82, .	3.2	4
25	Theoretical Investigations on the Healing of Monovacancies in Single-Walled Carbon Nanotubes by Adsorption of Carbon Monoxide. Journal of Physical Chemistry C, 2010, 114, 21322-21326.	3.1	8
26	Unraveling the Reactivity of Semiconducting Chiral Carbon Nanotubes through Finite-Length Models Based on Clar Sextet Theory. Journal of Physical Chemistry C, 2009, 113, 862-866.	3.1	26
27	Theoretical Investigations of the Relaxation and Reconstruction of the Î³-AlO(OH) Boehmite (101) Surface and Boehmite Nanorods. Journal of Physical Chemistry C, 2009, 113, 5228-5237.	3.1	23
28	First-principles investigations on the functionalization of chiral and non-chiral carbon nanotubes by Dielsâ€“Alder cycloaddition reactions. Physical Chemistry Chemical Physics, 2009, 11, 563-567.	2.8	25
29	Electronic properties and stability of graphene nanoribbons: An interpretation based on Clar sextet theory. Chemical Physics Letters, 2008, 464, 202-207.	2.6	81
30	Semiempirical calculations on the electronic properties of finite-length models of carbon nanotubes based on Clar sextet theory. Molecular Simulation, 2008, 34, 905-908.	2.0	5
31	Finite-Length Models of Carbon Nanotubes Based on Clar Sextet Theory. Organic Letters, 2007, 9, 4267-4270.	4.6	53
32	Theoretical investigations on the functionalization of carbon nanotubes. Inorganica Chimica Acta, 2007, 360, 785-793.	2.4	28
33	Vacancy-Induced Chemisorption of NO2on Carbon Nanotubes:Â A Combined Theoretical and Experimental Study. Journal of Physical Chemistry B, 2005, 109, 13175-13179.	2.6	44
34	Role of defects on the gas sensing properties of carbon nanotubes thin films: experiment and theory. Chemical Physics Letters, 2004, 387, 356-361.	2.6	121
35	Influence of substituents and length of silanylene units on the electronic structure of Ï€ -conjugated polymeric organosilicon systems. Computational and Theoretical Chemistry, 1999, 489, 35-41.	1.5	9