

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	Role of defects on the gas sensing properties of carbon nanotubes thin films: experiment and theory. <i>Chemical Physics Letters</i> , 2004, 387, 356-361.	2.6	121
2	Electronic properties and stability of graphene nanoribbons: An interpretation based on Clar sextet theory. <i>Chemical Physics Letters</i> , 2008, 464, 202-207.	2.6	81
3	High-Performance and Stable Perovskite Solar Cells Based on Dopant-Free Arylamine-Substituted Copper(II) Phthalocyanine Hole-Transporting Materials. <i>Advanced Energy Materials</i> , 2019, 9, 1901019.	19.5	80
4	Finite-Length Models of Carbon Nanotubes Based on Clar Sextet Theory. <i>Organic Letters</i> , 2007, 9, 4267-4270.	4.6	53
5	Vacancy-Induced Chemisorption of NO ₂ on Carbon Nanotubes: A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 13175-13179.	2.6	44
6	Toward Real Setting Applications of Organic and Perovskite Solar Cells: A Comparative Review. <i>Energy Technology</i> , 2021, 9, 2000901.	3.8	33
7	Theoretical investigations on the functionalization of carbon nanotubes. <i>Inorganica Chimica Acta</i> , 2007, 360, 785-793.	2.4	28
8	Towards nano-organic chemistry: perspectives for a bottom-up approach to the synthesis of low-dimensional carbon nanostructures. <i>Nanoscale</i> , 2012, 4, 369-379.	5.6	27
9	Unraveling the Reactivity of Semiconducting Chiral Carbon Nanotubes through Finite-Length Models Based on Clar Sextet Theory. <i>Journal of Physical Chemistry C</i> , 2009, 113, 862-866.	3.1	26
10	First-principles investigations on the functionalization of chiral and non-chiral carbon nanotubes by Diels-Alder cycloaddition reactions. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 563-567.	2.8	25
11	Theoretical Investigations of the Relaxation and Reconstruction of the $\hat{\Gamma}^3$ -AlO(OH) Boehmite (101) Surface and Boehmite Nanorods. <i>Journal of Physical Chemistry C</i> , 2009, 113, 5228-5237.	3.1	23
12	A Structural Model of a P450-Ferredoxin Complex from Orientation-Selective Double Electron-Electron Resonance Spectroscopy. <i>Journal of the American Chemical Society</i> , 2018, 140, 2514-2527.	13.7	22
13	Correlation between gate-dielectric morphology at the nanoscale and charge transport properties in organic field-effect transistors. <i>RSC Advances</i> , 2015, 5, 11797-11805.	3.6	15
14	Morphology and Electronic Properties of <i>N,N</i> -Ditridecylperylene-3,4,9,10-tetracarboxylic Diimide Layered Aggregates: From Structural Predictions to Charge Transport. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21857-21864.	3.1	14
15	Nanoscale morphology and electronic coupling at the interface between indium tin oxide and organic molecular materials. <i>Nanoscale</i> , 2018, 10, 9376-9385.	5.6	14
16	Epitaxial multilayers of alkanes on two-dimensional black phosphorus as passivating and electrically insulating nanostructures. <i>Nanoscale</i> , 2019, 11, 17252-17261.	5.6	13
17	Redox-switchable devices based on functionalized graphene nanoribbons. <i>Nanoscale</i> , 2012, 4, 1350.	5.6	12
18	Theoretical insights on morphology and charge transport properties of two-dimensional <i>N,N</i> -ditridecylperylene-3,4,9,10-tetra carboxylic diimide aggregates. <i>RSC Advances</i> , 2016, 6, 40724-40730.	3.6	11

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19	Stiffness of Fluid and Gel Phase Lipid Nanovesicles: Weighting the Contributions of Membrane Bending Modulus and Luminal Pressurization. <i>Langmuir</i> , 2021, 37, 12027-12037.	3.5	10
20	Influence of substituents and length of silanylene units on the electronic structure of π -conjugated polymeric organosilicon systems. <i>Computational and Theoretical Chemistry</i> , 1999, 489, 35-41.	1.5	9
21	On the Nature of Charge-Injecting Contacts in Organic Field-Effect Transistors. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 30616-30626.	8.0	9
22	Theoretical Investigations on the Healing of Monovacancies in Single-Walled Carbon Nanotubes by Adsorption of Carbon Monoxide. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21322-21326.	3.1	8
23	A self-assembled lysinated perylene diimide film as a multifunctional material for neural interfacing. <i>Journal of Materials Chemistry B</i> , 2016, 4, 2921-2932.	5.8	8
24	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. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28393-28399.	2.8	8
25	A Computational Predictive Approach for Controlling the Morphology of Functional Molecular Aggregates on Substrates. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900156.	2.8	7
26	Correlation between atomistic morphology and electron transport properties in defect-free and defected graphene nanoribbons: An interpretation through Clar sextet theory. <i>Carbon</i> , 2014, 75, 190-200.	10.3	6
27	Evidence of benzenoid domains in nanographenes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2088-2093.	2.8	6
28	Noncovalent passivation of supported phosphorene for device applications: from morphology to electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12482-12488.	2.8	6
29	Semiempirical calculations on the electronic properties of finite-length models of carbon nanotubes based on Clar sextet theory. <i>Molecular Simulation</i> , 2008, 34, 905-908.	2.0	5
30	Synthesis and investigation on processing-depending polarized fluorescence emission in thin-films of 2,2'-([2,2'-bithiophene]-5,5'-diyl)bis(5-octyl-4-phenyl-4H-thieno[2,3-c]pyrrol-6(5H)-one). <i>Journal of Materials Chemistry C</i> , 2017, 5, 10320-10331.	5.5	5
31	Efficient evaluation of Coulomb interactions in kinetic Monte Carlo simulations of charge transport. <i>Journal of Chemical Physics</i> , 2020, 152, 164102.	3.0	5
32	A Molecular Drone for Atomic-Scale Fabrication Working under Ambient Conditions. <i>Advanced Materials</i> , 2021, 33, e2007150.	21.0	5
33	Modeling of low-dimensional carbon nanostructures: an efficient approach based on chemical criteria. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2010, 7, 2632-2635.	0.8	4
34	Atomistic engineering in the control of the electronic properties of CdSe nanotubes. <i>Physical Review B</i> , 2010, 82, .	3.2	4
35	3D versus 2D Electrolyte-Semiconductor Interfaces in Rylene-diimide-Based Electron-Transporting Water-Gated Organic Field-Effect Transistors. <i>Advanced Electronic Materials</i> , 2020, 6, 2000638.	5.1	2