

Daniele Meggiolaro

List of Publications by Year in descending order

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39
papers

4,568
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186265
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citing authors

#	ARTICLE	IF	CITATIONS
1	Role of Terminal Group Position in Triphenylamine-Based Self-Assembled Hole-Selective Molecules in Perovskite Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 17461-17469.	8.0	15
2	Tuning halide perovskite energy levels. <i>Energy and Environmental Science</i> , 2021, 14, 1429-1438.	30.8	124
3	Halide-driven formation of lead halide perovskites: insight from <i>ab initio</i> molecular dynamics simulations. <i>Materials Advances</i> , 2021, 2, 3915-3926.	5.4	18
4	Composition-Dependent Struggle between Iodine and Tin Chemistry at the Surface of Mixed Tin/Lead Perovskites. <i>ACS Energy Letters</i> , 2021, 6, 969-976.	17.4	27
5	Energy vs Charge Transfer in Manganese-Doped Lead Halide Perovskites. <i>ACS Energy Letters</i> , 2021, 6, 1869-1878.	17.4	36
6	Large Cation Engineering in Two-Dimensional Silver-Bismuth Bromide Double Perovskites. <i>Chemistry of Materials</i> , 2021, 33, 4688-4700.	6.7	25
7	Suppression of Tin Oxidation by 3D/2D Perovskite Interfacing. <i>Journal of Physical Chemistry C</i> , 2021, 125, 10901-10908.	3.1	15
8	Defect activity in metal halide perovskites with wide and narrow bandgap. <i>Nature Reviews Materials</i> , 2021, 6, 986-1002.	48.7	121
9	Brightly Luminescent and Moisture Tolerant Phenyl Viologen Lead Iodide Perovskites for Light Emission Applications. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5456-5462.	4.6	5
10	Halogen-Bonded Hole-Transport Material Suppresses Charge Recombination and Enhances Stability of Perovskite Solar Cells. <i>Advanced Energy Materials</i> , 2021, 11, 2101553.	19.5	44
11	<i>In situ</i> cadmium surface passivation of perovskite nanocrystals for blue LEDs. <i>Journal of Materials Chemistry A</i> , 2021, 9, 26750-26757.	10.3	18
12	The Doping Mechanism of Halide Perovskite Unveiled by Alkaline Earth Metals. <i>Journal of the American Chemical Society</i> , 2020, 142, 2364-2374.	13.7	132
13	Modulating Band Alignment in Mixed Dimensionality 3D/2D Perovskites by Surface Termination Ligand Engineering. <i>Chemistry of Materials</i> , 2020, 32, 105-113.	6.7	19
14	Polarons in Metal Halide Perovskites. <i>Advanced Energy Materials</i> , 2020, 10, 1902748.	19.5	84
15	Lanthanide-Induced Photoluminescence in Lead-Free Cs ₂ AgBiBr ₆ Bulk Perovskite: Insights from Optical and Theoretical Investigations. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8893-8900.	4.6	38
16	Formation of Color Centers in Lead Iodide Perovskites: Self-Trapping and Defects in the Bulk and Surfaces. <i>Chemistry of Materials</i> , 2020, 32, 6916-6924.	6.7	23
17	Instability of Tin Iodide Perovskites: Bulk p-Doping versus Surface Tin Oxidation. <i>ACS Energy Letters</i> , 2020, 5, 2787-2795.	17.4	143
18	Charge localization and trapping at surfaces in lead-iodide perovskites: the role of polarons and defects. <i>Journal of Materials Chemistry A</i> , 2020, 8, 6882-6892.	10.3	49

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19	Coupling halide perovskites with different materials: From doping to nanocomposites, beyond photovoltaics. <i>Progress in Materials Science</i> , 2020, 110, 100639.	32.8	38
20	Tin versus Lead Redox Chemistry Modulates Charge Trapping and Self-Doping in Tin/Lead Iodide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3546-3556.	4.6	132
21	Charge Carriers Are Not Affected by the Relatively Slow-Rotating Methylammonium Cations in Lead Halide Perovskite Thin Films. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5128-5134.	4.6	16
22	Energy Level Tuning at the MAPbI ₃ Perovskite/Contact Interface Using Chemical Treatment. <i>ACS Energy Letters</i> , 2019, 4, 2181-2184.	17.4	45
23	Defect Activity in Lead Halide Perovskites. <i>Advanced Materials</i> , 2019, 31, e1901183.	21.0	191
24	Charge Localization, Stabilization, and Hopping in Lead Halide Perovskites: Competition between Polaron Stabilization and Cation Disorder. <i>ACS Energy Letters</i> , 2019, 4, 2013-2020.	17.4	43
25	The nature of the lead-iodine bond in PbI ₂ : A case study for the modelling of lead halide perovskites. <i>Computational and Theoretical Chemistry</i> , 2019, 1164, 112558.	2.5	9
26	Controlling competing photochemical reactions stabilizes perovskite solar cells. <i>Nature Photonics</i> , 2019, 13, 532-539.	31.4	273
27	Electrochemical Hole Injection Selectively Expels Iodide from Mixed Halide Perovskite Films. <i>Journal of the American Chemical Society</i> , 2019, 141, 10812-10820.	13.7	104
28	Ultrafast THz Probe of Photoinduced Polarons in Lead-Halide Perovskites. <i>Physical Review Letters</i> , 2019, 122, 166601.	7.8	98
29	From Large to Small Polarons in Lead, Tin, and Mixed Lead-Tin Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1790-1798.	4.6	72
30	Formation of Surface Defects Dominates Ion Migration in Lead-Halide Perovskites. <i>ACS Energy Letters</i> , 2019, 4, 779-785.	17.4	219
31	Modeling the Interaction of Molecular Iodine with MAPbI ₃ : A Probe of Lead-Halide Perovskites Defect Chemistry. <i>ACS Energy Letters</i> , 2018, 3, 447-451.	17.4	88
32	Iodine chemistry determines the defect tolerance of lead-halide perovskites. <i>Energy and Environmental Science</i> , 2018, 11, 702-713.	30.8	480
33	First-Principles Modeling of Bismuth Doping in the MAPbI ₃ Perovskite. <i>Journal of Physical Chemistry C</i> , 2018, 122, 14107-14112.	3.1	64
34	First-Principles Modeling of Defects in Lead Halide Perovskites: Best Practices and Open Issues. <i>ACS Energy Letters</i> , 2018, 3, 2206-2222.	17.4	202
35	Broadband Emission in Two-Dimensional Hybrid Perovskites: The Role of Structural Deformation. <i>Journal of the American Chemical Society</i> , 2017, 139, 39-42.	13.7	336
36	Fluorescent Alloy CsPb _x Mn _{1-x} I ₃ Perovskite Nanocrystals with High Structural and Optical Stability. <i>ACS Energy Letters</i> , 2017, 2, 2183-2186.	17.4	305

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37	Large polarons in lead halide perovskites. <i>Science Advances</i> , 2017, 3, e1701217.	10.3	515
38	Mechanism of Reversible Trap Passivation by Molecular Oxygen in Lead-Halide Perovskites. <i>ACS Energy Letters</i> , 2017, 2, 2794-2798.	17.4	100
39	Light-induced annihilation of Frenkel defects in organo-lead halide perovskites. <i>Energy and Environmental Science</i> , 2016, 9, 3180-3187.	30.8	302