Francesco Ambrosio

List of Publications by Year
in descending order

42 papers	1,866 citations	218677 26 h-index	276875 41 g-index
44 all docs	44 docs citations	44 times ranked	2550 citing authors

#	Article	IF	Citations
1	Charge Localization in Defective BiVO₄. Journal of Physical Chemistry C, 2022, 126, 2960-2970.	3.1	14
2	Effect of electronic doping and traps on carrier dynamics in tin halide perovskites. Materials Horizons, 2022, 9, 1763-1773.	12.2	23
3	Reaction Mechanism of Photocatalytic Hydrogen Production at Water/Tin Halide Perovskite Interfaces. ACS Energy Letters, 2022, 7, 1308-1315.	17.4	26
4	Stability of Tin- versus Lead-Halide Perovskites: Ab Initio Molecular Dynamics Simulations of Perovskite/Water Interfaces. Journal of Physical Chemistry Letters, 2022, 13, 2321-2329.	4.6	29
5	Waterâ€Stable DMASnBr₃ Leadâ€Free Perovskite for Effective Solarâ€Driven Photocatalysis. Angewandte Chemie - International Edition, 2021, 60, 3611-3618.	13.8	72
6	Waterâ€Stable DMASnBr₃ Leadâ€Free Perovskite for Effective Solarâ€Driven Photocatalysis. Angewandte Chemie, 2021, 133, 3655-3662.	2.0	12
7	Composition-Dependent Struggle between Iodine and Tin Chemistry at the Surface of Mixed Tin/Lead Perovskites. ACS Energy Letters, 2021, 6, 969-976.	17.4	27
8	Strong Electron Localization in Tin Halide Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 5339-5343.	4.6	22
9	Experimental Strategy and Mechanistic View to Boost the Photocatalytic Activity of Cs₃Bi₂Br₉ Leadâ€Free Perovskite Derivative by gâ€C₃N₄ Composite Engineering. Advanced Functional Materials, 2021, 31, 2104428.	14.9	53
10	Polarons in Metal Halide Perovskites. Advanced Energy Materials, 2020, 10, 1902748.	19.5	84
11	Formation of Color Centers in Lead Iodide Perovskites: Self-Trapping and Defects in the Bulk and Surfaces. Chemistry of Materials, 2020, 32, 6916-6924.	6.7	23
12	Combined Computational and Experimental Investigation on the Nature of Hydrated Iodoplumbate Complexes: Insights into the Dual Role of Water in Perovskite Precursor Solutions. Journal of Physical Chemistry B, 2020, 124, 11481-11490.	2.6	21
13	Instability of Tin Iodide Perovskites: Bulk p-Doping versus Surface Tin Oxidation. ACS Energy Letters, 2020, 5, 2787-2795.	17.4	143
14	Evaluation of Photocatalysts for Water Splitting through Combined Analysis of Surface Coverage and Energy-Level Alignment. ACS Catalysis, 2020, 10, 13186-13195.	11.2	19
15	Charge localization and trapping at surfaces in lead-iodide perovskites: the role of polarons and defects. Journal of Materials Chemistry A, 2020, 8, 6882-6892.	10.3	49
16	On the Electronic and Optical Properties of Metalâ€“Organic Frameworks: Case Study of MIL-125 and MIL-125-NH₂. Journal of Physical Chemistry C, 2020, 124, 4065-4072.	3.1	50
17	Effect of the Solvent on the Oxygen Evolution Reaction at the TiO₂â€“Water Interface. Journal of Physical Chemistry C, 2019, 123, 18467-18474.	3.1	25
18	Charge Localization, Stabilization, and Hopping in Lead Halide Perovskites: Competition between Polaron Stabilization and Cation Disorder. ACS Energy Letters, 2019, 4, 2013-2020.	17.4	43

#	Article	IF	Citations
19	Picture of the wet electron: a localized transient state in liquid water. Chemical Science, 2019, 10, 7442-7448.	7.4	43
20	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. Npj Computational Materials, 2019, 5, .	8.7	48
21	Strong Hole Trapping Due to Oxygen Dimers in BiVO₄: Effect on the Water Oxidation Reaction. Journal of Physical Chemistry Letters, 2019, 10, 7113-7118.	4.6	13
22	Extrinsic Defects in Amorphous Oxides: Hydrogen, Carbon, and Nitrogen Impurities in Alumina. Physical Review Applied, 2019, 11, .	3.8	7
23	pH-Dependent Catalytic Reaction Pathway for Water Splitting at the BiVO₄â€“Water Interface from the Band Alignment. ACS Energy Letters, 2018, 3, 829-834.	17.4	41
24	pH-Dependent Surface Chemistry from First Principles: Application to the BiVO₄(010)â€“Water Interface. ACS Applied Materials & Interfaces, 2018, 10, 10011-10021.	8.0	46
25	Origin of low electronâ€“hole recombination rate in metal halide perovskites. Energy and Environmental Science, 2018, 11, 101-105.	30.8	113
26	Alignment of Redox Levels at Semiconductorâ€“Water Interfaces. Chemistry of Materials, 2018, 30, 94-111.	6.7	74
27	Reactivity and energy level of a localized hole in liquid water. Physical Chemistry Chemical Physics, 2018, 20, 30281-30289.	2.8	10
28	Absolute Energy Levels of Liquid Water. Journal of Physical Chemistry Letters, 2018, 9, 3212-3216.	4.6	51
29	Hole diffusion across leaky amorphous TiO₂coating layers for catalytic water splitting at photoanodes. Journal of Materials Chemistry A, 2018, 6, 11804-11810.	10.3	18
30	Surface Polarons Reducing Overpotentials in the Oxygen Evolution Reaction. ACS Catalysis, 2018, 8, 5847-5851.	11.2	37
31	Role of Polarons in Water Splitting: The Case of BiVO₄. ACS Energy Letters, 2018, 3, 1693-1697.	17.4	65
32	Mechanism suppressing charge recombination at iodine defects in CH3NH3PbI3 by polaron formation. Journal of Materials Chemistry A, 2018, 6, 16863-16867.	10.3	26
33	Electronic Levels of Excess Electrons in Liquid Water. Journal of Physical Chemistry Letters, 2017, 8, 2055-2059.	4.6	70
34	Note: Assessment of the SCAN+rVV10 functional for the structure of liquid water. Journal of Chemical Physics, 2017, 147, 216101.	3.0	30
35	Comprehensive modeling of the band gap and absorption spectrum of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiVO</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> Physical Review Materials, 2017, 1, .	2.4	44
36	Oxygen defects in amorphous Al2O3: A hybrid functional study. Applied Physics Letters, 2016, 109, .	3.3	41

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37	Structural, Dynamical, and Electronic Properties of Liquid Water: A Hybrid Functional Study. Journal of Physical Chemistry B, 2016, 120, 7456-7470.	2.6	61
38	AbÂinitio Electronic Structure of Liquid Water. Physical Review Letters, 2016, 117, 186401.	7.8	64
39	Redox levels in aqueous solution: Effect of van der Waals interactions and hybrid functionals. Journal of Chemical Physics, 2015, 143, 244508.	3.0	62
40	Singlet fission in linear chains of molecules. Journal of Chemical Physics, 2014, 141, 204703.	3.0	16
41	What Is the Best Anchoring Group for a Dye in a Dye-Sensitized Solar Cell?. Journal of Physical Chemistry Letters, 2012, 3, 1531-1535.	4.6	151
42	(In-)Stability of Tin Halide Perovskites: Ab Initio Molecular Dynamics Simulations of Perovskite/Water Interfaces. , 0, , .		0