

Edoardo Mosconi

List of Publications by Year in descending order

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133
papers

23,987
citations

18482
62
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138
times ranked

19061
citing authors

#	ARTICLE	IF	CITATIONS
1	Intrinsic Thermal Instability of Methylammonium Lead Trihalide Perovskite. <i>Advanced Energy Materials</i> , 2015, 5, 1500477.	19.5	1,788
2	One-Year stable perovskite solar cells by 2D/3D interface engineering. <i>Nature Communications</i> , 2017, 8, 15684.	12.8	1,625
3	Defect migration in methylammonium lead iodide and its role in perovskite solar cell operation. <i>Energy and Environmental Science</i> , 2015, 8, 2118-2127.	30.8	1,278
4	Relativistic GW calculations on CH ₃ NH ₃ PbI ₃ and CH ₃ NH ₃ SnI ₃ Perovskites for Solar Cell Applications. <i>Scientific Reports</i> , 2014, 4, 4467.	3.3	1,093
5	Cation-Induced Band-Gap Tuning in Organohalide Perovskites: Interplay of Spin-Orbit Coupling and Octahedra Tilting. <i>Nano Letters</i> , 2014, 14, 3608-3616.	9.1	1,033
6	First-Principles Modeling of Mixed Halide Organometal Perovskites for Photovoltaic Applications. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13902-13913.	3.1	861
7	A molecularly engineered hole-transporting material for efficient perovskite solar cells. <i>Nature Energy</i> , 2016, 1, .	39.5	816
8	Solution Synthesis Approach to Colloidal Cesium Lead Halide Perovskite Nanoplatelets with Monolayer-Level Thickness Control. <i>Journal of the American Chemical Society</i> , 2016, 138, 1010-1016.	13.7	747
9	MAPbI _{3-x} Cl _x Mixed Halide Perovskite for Hybrid Solar Cells: The Role of Chloride as Dopant on the Transport and Structural Properties. <i>Chemistry of Materials</i> , 2013, 25, 4613-4618.	6.7	732
10	Stabilizing halide perovskite surfaces for solar cell operation with wide-bandgap lead oxysalts. <i>Science</i> , 2019, 365, 473-478.	12.6	723
11	The Raman Spectrum of the CH ₃ NH ₃ PbI ₃ Hybrid Perovskite: Interplay of Theory and Experiment. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 279-284.	4.6	555
12	Origin of the Thermal Instability in CH ₃ NH ₃ PbI ₃ Thin Films Deposited on ZnO. <i>Chemistry of Materials</i> , 2015, 27, 4229-4236.	6.7	548
13	Large polarons in lead halide perovskites. <i>Science Advances</i> , 2017, 3, e1701217.	10.3	515
14	Nearly Monodisperse Insulator Cs ₄ PbX ₆ (X = Cl, Br, I) Nanocrystals, Their Mixed Halide Compositions, and Their Transformation into CsPbX ₃ Nanocrystals. <i>Nano Letters</i> , 2017, 17, 1924-1930.	9.1	488
15	Iodine chemistry determines the defect tolerance of lead-halide perovskites. <i>Energy and Environmental Science</i> , 2018, 11, 702-713.	30.8	480
16	Ligand-engineered bandgap stability in mixed-halide perovskite LEDs. <i>Nature</i> , 2021, 591, 72-77.	27.8	471
17	Defect-Assisted Photoinduced Halide Segregation in Mixed-Halide Perovskite Thin Films. <i>ACS Energy Letters</i> , 2017, 2, 1416-1424.	17.4	437
18	Structural and optical properties of methylammonium lead iodide across the tetragonal to cubic phase transition: implications for perovskite solar cells. <i>Energy and Environmental Science</i> , 2016, 9, 155-163.	30.8	423

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19	<i>Ab Initio</i> Molecular Dynamics Simulations of Methylammonium Lead Iodide Perovskite Degradation by Water. <i>Chemistry of Materials</i> , 2015, 27, 4885-4892.	6.7	414
20	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
21	A Computational Investigation of Organic Dyes for Dye-Sensitized Solar Cells: Benchmark, Strategies, and Open Issues. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7205-7212.	3.1	328
22	Light-induced annihilation of Frenkel defects in organo-lead halide perovskites. <i>Energy and Environmental Science</i> , 2016, 9, 3180-3187.	30.8	302
23	Extremely Slow Photoconductivity Response of CH ₃ NH ₃ PbI ₃ Perovskites Suggesting Structural Changes under Working Conditions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2662-2669.	4.6	301
24	Interplay of Orientational Order and Electronic Structure in Methylammonium Lead Iodide: Implications for Solar Cell Operation. <i>Chemistry of Materials</i> , 2014, 26, 6557-6569.	6.7	286
25	Dynamical Origin of the Rashba Effect in Organohalide Lead Perovskites: A Key to Suppressed Carrier Recombination in Perovskite Solar Cells?. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1638-1645.	4.6	278
26	Controlling competing photochemical reactions stabilizes perovskite solar cells. <i>Nature Photonics</i> , 2019, 13, 532-539.	31.4	273
27	First-Principles Investigation of the TiO ₂ /Organohalide Perovskites Interface: The Role of Interfacial Chlorine. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2619-2625.	4.6	247
28	High Open-Circuit Voltage Solid-State Dye-Sensitized Solar Cells with Organic Dye. <i>Nano Letters</i> , 2009, 9, 2487-2492.	9.1	228
29	Absorption Spectra and Excited State Energy Levels of the N719 Dye on TiO ₂ in Dye-Sensitized Solar Cell Models. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8825-8831.	3.1	222
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	Structural and electronic properties of organo-halide lead perovskites: a combined IR-spectroscopy and ab initio molecular dynamics investigation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16137-16144.	2.8	211
32	Cobalt Electrolyte/Dye Interactions in Dye-Sensitized Solar Cells: A Combined Computational and Experimental Study. <i>Journal of the American Chemical Society</i> , 2012, 134, 19438-19453.	13.7	204
33	Stark Effect in Perovskite/TiO ₂ Solar Cells: Evidence of Local Interfacial Order. <i>Nano Letters</i> , 2014, 14, 2168-2174.	9.1	200
34	CH ₃ NH ₃ PbI ₃ perovskite single crystals: surface photophysics and their interaction with the environment. <i>Chemical Science</i> , 2015, 6, 7305-7310.	7.4	192
35	Photoinduced Reversible Structural Transformations in Free-Standing CH ₃ NH ₃ PbI ₃ Perovskite Films. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2332-2338.	4.6	190
36	Di-branched di-anchoring organic dyes for dye-sensitized solar cells. <i>Energy and Environmental Science</i> , 2009, 2, 1094.	30.8	188

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37	Intrinsic Halide Segregation at Nanometer Scale Determines the High Efficiency of Mixed Cation/Mixed Halide Perovskite Solar Cells. <i>Journal of the American Chemical Society</i> , 2016, 138, 15821-15824.	13.7	179
38	Mobile Ions in Organohalide Perovskites: Interplay of Electronic Structure and Dynamics. <i>ACS Energy Letters</i> , 2016, 1, 182-188.	17.4	179
39	Elusive Presence of Chloride in Mixed Halide Perovskite Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3532-3538.	4.6	175
40	Electronic and optical properties of mixed Sn/Pb organohalide perovskites: a first principles investigation. <i>Journal of Materials Chemistry A</i> , 2015, 3, 9208-9215.	10.3	170
41	Adsorption of organic dyes on TiO ₂ surfaces in dye-sensitized solar cells: interplay of theory and experiment. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15963.	2.8	151
42	Ionotronic Halide Perovskite Drift-Diffusive Synapses for Low-Power Neuromorphic Computation. <i>Advanced Materials</i> , 2018, 30, e1805454.	21.0	146
43	Electronic and optical properties of MAPbX ₃ perovskites (X = I, Br, Cl): a unified DFT and GW theoretical analysis. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27158-27164.	2.8	140
44	Large electrostrictive response in lead halide perovskites. <i>Nature Materials</i> , 2018, 17, 1020-1026.	27.5	137
45	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
46	Structural and electronic properties of organo-halide hybrid perovskites from ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9394-9409.	2.8	130
47	High Open-Circuit Voltage: Fabrication of Formamidinium Lead Bromide Perovskite Solar Cells Using Fluorene-Dithiophene Derivatives as Hole-Transporting Materials. <i>ACS Energy Letters</i> , 2016, 1, 107-112.	17.4	105
48	Rashba Band Splitting in Organohalide Lead Perovskites: Bulk and Surface Effects. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2247-2252.	4.6	101
49	Mechanism of Reversible Trap Passivation by Molecular Oxygen in Lead-Halide Perovskites. <i>ACS Energy Letters</i> , 2017, 2, 2794-2798.	17.4	100
50	Tuning structural isomers of phenylenediammonium to afford efficient and stable perovskite solar cells and modules. <i>Nature Communications</i> , 2021, 12, 6394.	12.8	98
51	Understanding Performance Limiting Interfacial Recombination in <i>pin</i> Perovskite Solar Cells. <i>Advanced Energy Materials</i> , 2022, 12, .	19.5	95
52	Infrared Dielectric Screening Determines the Low Exciton Binding Energy of Metal-Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 620-627.	4.6	88
53	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
54	Computational Investigation of Dye-Iodine Interactions in Organic Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5965-5973.	3.1	86

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55	Polarons in Metal Halide Perovskites. <i>Advanced Energy Materials</i> , 2020, 10, 1902748.	19.5	84
56	Solvent Effects on the Adsorption Geometry and Electronic Structure of Dye-Sensitized TiO ₂ : A First-Principles Investigation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5932-5940.	3.1	83
57	Supramolecular Interactions of Chenodeoxycholic Acid Increase the Efficiency of Dye-Sensitized Solar Cells Based on a Cobalt Electrolyte. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3874-3887.	3.1	82
58	Globularity-Selected Large Molecules for a New Generation of Multication Perovskites. <i>Advanced Materials</i> , 2017, 29, 1702005.	21.0	81
59	Inherent electronic trap states in TiO ₂ nanocrystals: effect of saturation and sintering. <i>Energy and Environmental Science</i> , 2013, 6, 1221.	30.8	76
60	Understanding the Solution Chemistry of Lead Halide Perovskites Precursors. <i>ACS Applied Energy Materials</i> , 2019, 2, 3400-3409.	5.1	74
61	Water-Stable DMASnBr ₃ Lead-Free Perovskite for Effective Solar-Driven Photocatalysis. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 3611-3618.	13.8	72
62	Water Oxidation by the [Co ₄ O ₄ (OAc) ₄ (py) ₄] ⁺ Cubium is Initiated by OH ⁻ Addition. <i>Journal of the American Chemical Society</i> , 2015, 137, 15460-15468.	13.7	64
63	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
64	Enhanced TiO ₂ /MAPbI ₃ Electronic Coupling by Interface Modification with PbI ₂ . <i>Chemistry of Materials</i> , 2016, 28, 3612-3615.	6.7	60
65	Long-Lived Photoinduced Polarons in Organohalide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3081-3086.	4.6	59
66	Solvent-Free Synthetic Route for Cerium(IV) Metal-Organic Frameworks with UiO-66 Architecture and Their Photocatalytic Applications. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 45031-45037.	8.0	58
67	Band Gap Engineering in MASnBr ₃ and CsSnBr ₃ Perovskites: Mechanistic Insights through the Application of Pressure. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7398-7405.	4.6	57
68	Surface Reconstruction Engineering with Synergistic Effect of Mixed-Salt Passivation Treatment toward Efficient and Stable Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2021, 31, 2102902.	14.9	57
69	Modeling ZnS and ZnO Nanostructures: Structural, Electronic, and Optical Properties. <i>Journal of Physical Chemistry C</i> , 2011, 115, 25219-25226.	3.1	56
70	Rationalizing the Molecular Design of Hole-Selective Contacts to Improve Charge Extraction in Perovskite Solar Cells. <i>Advanced Energy Materials</i> , 2019, 9, 1900990.	19.5	56
71	Experimental Strategy and Mechanistic View to Boost the Photocatalytic Activity of Cs ₃ Bi ₂ Br ₉ Lead-Free Perovskite Derivative by g-C ₃ N ₄ Composite Engineering. <i>Advanced Functional Materials</i> , 2021, 31, 2104428.	14.9	53
72	Electronic structure of MAPbI ₃ and MAPbCl ₃ : importance of band alignment. <i>Scientific Reports</i> , 2019, 9, 15159.	3.3	52

73	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
74	Outstanding Passivation Effect by a Mixed-Salt Interlayer with Internal Interactions in Perovskite Solar Cells. <i>ACS Energy Letters</i> , 2020, 5, 3159-3167.	17.4	47
75	Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface. <i>ACS Energy Letters</i> , 2016, 1, 454-463.	17.4	46
76	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
77	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
78	Chlorine Incorporation in the CH ₃ NH ₃ PbI ₃ Perovskite: Small Concentration, Big Effect. <i>Inorganic Chemistry</i> , 2017, 56, 74-83.	4.0	40
79	New Fullerene Derivative as an n-Type Material for Highly Efficient, Flexible Perovskite Solar Cells of a p-n Configuration. <i>Advanced Functional Materials</i> , 2020, 30, 2004357.	14.9	38
80	An Oxa[5]helicene-Based Racemic Semiconducting Glassy Film for Photothermally Stable Perovskite Solar Cells. <i>IScience</i> , 2019, 15, 234-242.	4.1	36
81	Energy vs Charge Transfer in Manganese-Doped Lead Halide Perovskites. <i>ACS Energy Letters</i> , 2021, 6, 1869-1878.	17.4	36
82	Large-scale GW -BSE calculations with N^3 scaling: Excitonic effects in dye-sensitized solar cells. <i>Physical Review B</i> , 2017, 95, .	3.2	34
83	First principles modelling of perovskite solar cells based on TiO ₂ and Al ₂ O ₃ : stability and interfacial electronic structure. <i>Journal of Materials Chemistry A</i> , 2017, 5, 2339-2345.	10.3	34
84	Influence of Disorder and Anharmonic Fluctuations on the Dynamical Rashba Effect in Purely Inorganic Lead-Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2019, 123, 291-298.	3.1	32
85	Exploring the Limits of Three-Dimensional Perovskites: The Case of FAPbI ₃ SnBr ₃ . <i>ACS Energy Letters</i> , 2018, 3, 1353-1359.	17.4	31
86	Synthesis, Properties, and Modeling of Cs _{1-x} Rb _x SnBr ₃ Solid Solution: A New Mixed-Cation Lead-Free All-Inorganic Perovskite System. <i>Chemistry of Materials</i> , 2019, 31, 3527-3533.	6.7	30
87	From Experiments to a Fast Easy-to-Use Computational Methodology to Predict Human Aldehyde Oxidase Selectivity and Metabolic Reactions. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 360-371.	6.4	29
88	Stability of Tin- versus Lead-Halide Perovskites: Ab Initio Molecular Dynamics Simulations of Perovskite/Water Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2321-2329.	4.6	29
89	Pyridine-EDOT Heteroarylene-Vinylene Donor-Acceptor Polymers. <i>Macromolecules</i> , 2010, 43, 9698-9713.	4.8	28
90	Computational modeling of single- versus double-anchoring modes in di-branched organic sensitizers on TiO ₂ surfaces: structural and electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4709-4719.	2.8	28

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91	Computational Modeling of Isoindigo-Based Polymers Used in Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17940-17954.	3.1	27
92	Reaction Mechanism of Photocatalytic Hydrogen Production at Water/Tin Halide Perovskite Interfaces. <i>ACS Energy Letters</i> , 2022, 7, 1308-1315.	17.4	26
93	A vinylene-linked benzo[1,2-b:4,5-b']dithiophene-2,1,3-benzothiadiazole low-bandgap polymer. <i>Journal of Polymer Science Part A</i> , 2012, 50, 2829-2840.	2.3	25
94	Trends in Perovskite Solar Cells and Optoelectronics: Status of Research and Applications from the PSCO Conference. <i>ACS Energy Letters</i> , 2017, 2, 857-861.	17.4	25
95	Electronic Properties and Carrier Trapping in Bi and Mn Co-doped CsPbCl ₃ Perovskite. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5482-5489.	4.6	25
96	Transition Dipole Moments of n = 1, 2, and 3 Perovskite Quantum Wells from the Optical Stark Effect and Many-Body Perturbation Theory. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 716-723.	4.6	24
97	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
98	A new lead-free 1D hybrid copper perovskite and its structural, thermal, vibrational, optical and magnetic characterization. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5970-5976.	5.5	23
99	A new terpyridine cobalt complex redox shuttle for dye-sensitized solar cells. <i>Inorganica Chimica Acta</i> , 2013, 406, 106-112.	2.4	21
100	Thiocyanate-Free Ruthenium(II) Sensitizers for Dye-Sensitized Solar Cells Based on the Cobalt Redox Couple. <i>ChemSusChem</i> , 2014, 7, 2930-2938.	6.8	21
101	Effect of Molecular Fluctuations on Hole Diffusion within Dye Monolayers. <i>Chemistry of Materials</i> , 2014, 26, 4731-4740.	6.7	21
102	Unveiling the nature of post-linear response Z-vector method for time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2017, 147, 024108.	3.0	21
103	Combined Computational and Experimental Investigation on the Nature of Hydrated Iodoplumbate Complexes: Insights into the Dual Role of Water in Perovskite Precursor Solutions. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11481-11490.	2.6	21
104	Decoding ultrafast polarization responses in lead halide perovskites by the two-dimensional optical Kerr effect. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	21
105	Computational Investigations on Organic Sensitizers for Dye-Sensitized Solar Cell. <i>Current Organic Synthesis</i> , 2012, 9, 215-232.	1.3	20
106	Origin of pressure-induced band gap tuning in tin halide perovskites. <i>Materials Advances</i> , 2020, 1, 2840-2845.	5.4	20
107	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
108	Comparing the excited-state properties of a mixed-cation mixed-halide perovskite to methylammonium lead iodide. <i>Journal of Chemical Physics</i> , 2020, 152, 104703.	3.0	18

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109	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
110	Cation Engineering for Resonant Energy Level Alignment in Two-Dimensional Lead Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2528-2535.	4.6	17
111	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
112	Structural and Optical Properties of Solvated PbI_2 in γ -Butyrolactone: Insight into the Solution Chemistry of Lead Halide Perovskite Precursors. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6139-6145.	4.6	15
113	Merging of E2 and E1cb Reaction Mechanisms: A Combined Theoretical and Experimental Study. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 5501-5504.	2.4	13
114	Alignment of energy levels in dye/semiconductor interfaces by $\langle \mathbf{r} \rangle$ effects due to coadsorption of solvent molecules. <i>Physical Review B</i> , 2014, 90, .	4.6	13
115	First-Principles Molecular Dynamics in Metal-Halide Perovskites: Contrasting Generalized Gradient Approximation and Hybrid Functionals. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11886-11893.	4.6	13
116	Effect of Structural Dynamics on the Opto-Electronic Properties of Bare and Hydrated ZnS QDs. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3274-3284.	3.1	12
117	DFT Investigation of Ligand-Based Reduction of CO_2 to CO on an Anionic Niobium Nitride Complex: Reaction Mechanism and Role of the Na^+ Counterion. <i>Organometallics</i> , 2011, 30, 4838-4846.	2.3	11
118	Iodide vs Chloride: The Impact of Different Lead Halides on the Solution Chemistry of Perovskite Precursors. <i>ACS Applied Energy Materials</i> , 2021, 4, 9827-9835.	5.1	11
119	Optical and magnetic characterization of one-dimensional $\text{Cu}(\text{II})$ -based perovskite: a high UV-Vis-NIR absorber. <i>Journal of Materials Chemistry C</i> , 2021, 9, 17158-17166.	5.5	9
120	Boron Functionalization and Unusual B-C Bond Activation in Rhodium(III) and Iridium(III) Complexes with Diphenylbis(pyrazolylborate) Ligands (Ph_2Bp). <i>Organometallics</i> , 2013, 32, 3895-3902.	2.3	8
121	Dynamical Rashba Band Splitting in Hybrid Perovskites Modeled by Local Electric Fields. <i>Journal of Physical Chemistry C</i> , 2018, 122, 124-132.	3.1	8
122	Designing New Indene-Fullerene Derivatives as Electron-Transporting Materials for Flexible Perovskite Solar Cells. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27344-27353.	3.1	8
123	Thermal Fluctuations on Förster Resonance Energy Transfer in Dyadic Solar Cell Sensitizers: A Combined Ab Initio Molecular Dynamics and TDDFT Investigation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16490-16499.	3.1	6
124	Zn^{2+} and Cu^{2+} doping of one-dimensional lead-free hybrid perovskite ABX_3 for white light emission and green solar cell applications. <i>Materials Research Bulletin</i> , 2022, 151, 111819.	5.2	6
125	A DFT investigation of base-catalyzed β -elimination reactions in water solution for systems activated by the pyridine ring: Theory vs. experiment. <i>Chemical Physics Letters</i> , 2008, 460, 100-107.	2.6	5
126	DFT studies of β -elimination reactions in water solution with different bases: Theory vs experiment. <i>Computational and Theoretical Chemistry</i> , 2010, 940, 103-114.	1.5	4

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127	MAPbI _{3-x} Cl _x mixed halide perovskite for hybrid solar cells: the role of chloride as dopant on the transport and structural properties. Materials Research Society Symposia Proceedings, 2014, 1667, 41.	0.1	4
128	First-Principles Modeling of Organohalide Thin Films and Interfaces. , 2016, , 19-52.		4
129	Investigating Charge Dynamics in Halide Perovskite Sensitized Mesostructured Solar Cells. Materials Research Society Symposia Proceedings, 2014, 1667, 7.	0.1	2
130	Real Spaceâ€Real Time Evolution of Excitonic States Based on the Bethe-Salpeter Equation Method. Journal of Physical Chemistry Letters, 2021, 12, 7261-7269.	4.6	2
131	Chapter 8. First Principles Modeling of Perovskite Solar Cells: Interplay of Structural, Electronic and Dynamical Effects. RSC Energy and Environment Series, 2016, , 234-296.	0.5	2
132	Ultrafast THz Fingerprints of Large Polaron formation in Lead-Halide Perovskites. , 2018, , .		1
133	(In-)Stability of Tin Halide Perovskites: Ab Initio Molecular Dynamics Simulations of Perovskite/Water Interfaces. , 0, , .		0