Edoardo Mosconi

List of Publications by Year
in descending order

133 papers	23,987 citations	18436 62 h-index	12910 131 g-index
138 all docs	138 docs citations	138 times ranked	19061 citing authors

#	Article	IF	Citations
1	Intrinsic Thermal Instability of Methylammonium Lead Trihalide Perovskite. Advanced Energy Materials, 2015, 5, 1500477.	10.2	1,788
2	One-Year stable perovskite solar cells by 2D/3D interface engineering. Nature Communications, 2017, 8, 15684.	5.8	1,625
3	Defect migration in methylammonium lead iodide and its role in perovskite solar cell operation. Energy and Environmental Science, 2015, 8, 2118-2127.	15.6	1,278
4	Relativistic GW calculations on CH3NH3PbI3 and CH3NH3SnI3 Perovskites for Solar Cell Applications. Scientific Reports, 2014, 4, 4467.	1.6	1,093
5	Cation-Induced Band-Gap Tuning in Organohalide Perovskites: Interplay of Spinâ€“Orbit Coupling and Octahedra Tilting. Nano Letters, 2014, 14, 3608-3616.	4.5	1,033
6	First-Principles Modeling of Mixed Halide Organometal Perovskites for Photovoltaic Applications. Journal of Physical Chemistry C, 2013, 117, 13902-13913.	1.5	861
7	A molecularly engineered hole-transporting material for efficient perovskite solar cells. Nature Energy, 2016, 1, .	19.8	816
8	Solution Synthesis Approach to Colloidal Cesium Lead Halide Perovskite Nanoplatelets with Monolayer-Level Thickness Control. Journal of the American Chemical Society, 2016, 138, 1010-1016.	6.6	747
9	MAPbI_{3-x}Cl_{<i>x</i>} Mixed Halide Perovskite for Hybrid Solar Cells: The Role of Chloride as Dopant on the Transport and Structural Properties. Chemistry of Materials, 2013, 25, 4613-4618.	3.2	732
10	Stabilizing halide perovskite surfaces for solar cell operation with wide-bandgap lead oxysalts. Science, 2019, 365, 473-478.	6.0	723
11	The Raman Spectrum of the CH₃NH₃PbI₃ Hybrid Perovskite: Interplay of Theory and Experiment. Journal of Physical Chemistry Letters, 2014, 5, 279-284.	2.1	555
12	Origin of the Thermal Instability in CH₃NH₃PbI₃ Thin Films Deposited on ZnO. Chemistry of Materials, 2015, 27, 4229-4236.	3.2	548
13	Large polarons in lead halide perovskites. Science Advances, 2017, 3, e1701217.	4.7	515
14	Nearly Monodisperse Insulator Cs₄PbX₆ (X = Cl, Br, I) Nanocrystals, Their Mixed Halide Compositions, and Their Transformation into CsPbX₃ Nanocrystals. Nano Letters, 2017, 17, 1924-1930.	4.5	488
15	Iodine chemistry determines the defect tolerance of lead-halide perovskites. Energy and Environmental Science, 2018, 11, 702-713.	15.6	480
16	Ligand-engineered bandgap stability in mixed-halide perovskite LEDs. Nature, 2021, 591, 72-77.	13.7	471
17	Defect-Assisted Photoinduced Halide Segregation in Mixed-Halide Perovskite Thin Films. ACS Energy Letters, 2017, 2, 1416-1424.	8.8	437
18	Structural and optical properties of methylammonium lead iodide across the tetragonal to cubic phase transition: implications for perovskite solar cells. Energy and Environmental Science, 2016, 9, 155-163.	15.6	423

#	ARTICLE	IF	CITATIONS
19	<i>Ab Initio</i> Molecular Dynamics Simulations of Methylammonium Lead Iodide Perovskite Degradation by Water. Chemistry of Materials, 2015, 27, 4885-4892.	3.2	414
20	Broadband Emission in Two-Dimensional Hybrid Perovskites: The Role of Structural Deformation. Journal of the American Chemical Society, 2017, 139, 39-42.	6.6	336
21	A Computational Investigation of Organic Dyes for Dye-Sensitized Solar Cells: Benchmark, Strategies, and Open Issues. Journal of Physical Chemistry C, 2010, 114, 7205-7212.	1.5	328
22	Light-induced annihilation of Frenkel defects in organo-lead halide perovskites. Energy and Environmental Science, 2016, 9, 3180-3187.	15.6	302
23	Extremely Slow Photoconductivity Response of CH₃NH₃PbI₃ Perovskites Suggesting Structural Changes under Working Conditions. Journal of Physical Chemistry Letters, 2014, 5, 2662-2669.	2.1	301
24	Interplay of Orientational Order and Electronic Structure in Methylammonium Lead Iodide: Implications for Solar Cell Operation. Chemistry of Materials, 2014, 26, 6557-6569.	3.2	286
25	Dynamical Origin of the Rashba Effect in Organohalide Lead Perovskites: A Key to Suppressed Carrier Recombination in Perovskite Solar Cells?. Journal of Physical Chemistry Letters, 2016, 7, 1638-1645.	2.1	278
26	Controlling competing photochemical reactions stabilizes perovskite solar cells. Nature Photonics, 2019, 13, 532-539.	15.6	273
27	First-Principles Investigation of the TiO₂/Organohalide Perovskites Interface: The Role of Interfacial Chlorine. Journal of Physical Chemistry Letters, 2014, 5, 2619-2625.	2.1	247
28	High Open-Circuit Voltage Solid-State Dye-Sensitized Solar Cells with Organic Dye. Nano Letters, 2009, 9, 2487-2492.	4.5	228
29	Absorption Spectra and Excited State Energy Levels of the N719 Dye on TiO₂ in Dye-Sensitized Solar Cell Models. Journal of Physical Chemistry C, 2011, 115, 8825-8831.	1.5	222
30	Formation of Surface Defects Dominates Ion Migration in Lead-Halide Perovskites. ACS Energy Letters, 2019, 4, 779-785.	8.8	219
31	Structural and electronic properties of organo-halide lead perovskites: a combined IR-spectroscopy and ab initio molecular dynamics investigation. Physical Chemistry Chemical Physics, 2014, 16, 16137-16144.	1.3	211
32	Cobalt Electrolyte/Dye Interactions in Dye-Sensitized Solar Cells: A Combined Computational and Experimental Study. Journal of the American Chemical Society, 2012, 134, 19438-19453.	6.6	204
33	Stark Effect in Perovskite/TiO₂ Solar Cells: Evidence of Local Interfacial Order. Nano Letters, 2014, 14, 2168-2174.	4.5	200
34	CH₃NH₃PbI₃ perovskite single crystals: surface photophysics and their interaction with the environment. Chemical Science, 2015, 6, 7305-7310.	3.7	192
35	Photoinduced Reversible Structural Transformations in Free-Standing CH₃NH₃PbI₃ Perovskite Films. Journal of Physical Chemistry Letters, 2015, 6, 2332-2338.	2.1	190
36	Di-branched di-anchoring organic dyes for dye-sensitized solar cells. Energy and Environmental Science, 2009, 2, 1094.	15.6	188

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37	Intrinsic Halide Segregation at Nanometer Scale Determines the High Efficiency of Mixed Cation/Mixed Halide Perovskite Solar Cells. Journal of the American Chemical Society, 2016, 138, 15821-15824.	6.6	179
38	Mobile Ions in Organohalide Perovskites: Interplay of Electronic Structure and Dynamics. ACS Energy Letters, 2016, 1, 182-188.	8.8	179
39	Elusive Presence of Chloride in Mixed Halide Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2014, 5, 3532-3538.	2.1	175
40	Electronic and optical properties of mixed Snâ€“Pb organohalide perovskites: a first principles investigation. Journal of Materials Chemistry A, 2015, 3, 9208-9215.	5.2	170
41	Adsorption of organic dyes on TiO2 surfaces in dye-sensitized solar cells: interplay of theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 15963.	1.3	151
42	Ionotronic Halide Perovskite Driftâ€Diffusive Synapses for Lowâ€Power Neuromorphic Computation. Advanced Materials, 2018, 30, e1805454.	11.1	146
43	Electronic and optical properties of MAPbX₃ perovskites (X = I, Br, Cl): a unified DFT and GW theoretical analysis. Physical Chemistry Chemical Physics, 2016, 18, 27158-27164.	1.3	140
44	Large electrostrictive response in lead halide perovskites. Nature Materials, 2018, 17, 1020-1026.	13.3	137
45	The Doping Mechanism of Halide Perovskite Unveiled by Alkaline Earth Metals. Journal of the American Chemical Society, 2020, 142, 2364-2374.	6.6	132
46	Structural and electronic properties of organo-halide hybrid perovskites from ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2015, 17, 9394-9409.	1.3	130
47	High Open-Circuit Voltage: Fabrication of Formamidinium Lead Bromide Perovskite Solar Cells Using Fluoreneâ€“Dithiophene Derivatives as Hole-Transporting Materials. ACS Energy Letters, 2016, 1, 107-112.	8.8	105
48	Rashba Band Splitting in Organohalide Lead Perovskites: Bulk and Surface Effects. Journal of Physical Chemistry Letters, 2017, 8, 2247-2252.	2.1	101
49	Mechanism of Reversible Trap Passivation by Molecular Oxygen in Lead-Halide Perovskites. ACS Energy Letters, 2017, 2, 2794-2798.	8.8	100
50	Tuning structural isomers of phenylenediammonium to afford efficient and stable perovskite solar cells and modules. Nature Communications, 2021, 12, 6394.	5.8	98
51	Understanding Performance Limiting Interfacial Recombination in <i>pin</i> Perovskite Solar Cells. Advanced Energy Materials, 2022, 12, .	10.2	95
52	Infrared Dielectric Screening Determines the Low Exciton Binding Energy of Metal-Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 620-627.	2.1	88
53	Modeling the Interaction of Molecular Iodine with MAPbI₃: A Probe of Lead-Halide Perovskites Defect Chemistry. ACS Energy Letters, 2018, 3, 447-451.	8.8	88
54	Computational Investigation of Dyeâ€“Iodine Interactions in Organic Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2012, 116, 5965-5973.	1.5	86

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55	Polarons in Metal Halide Perovskites. Advanced Energy Materials, 2020, 10, 1902748.	10.2	84
56	Solvent Effects on the Adsorption Geometry and Electronic Structure of Dye-Sensitized TiO₂: A First-Principles Investigation. Journal of Physical Chemistry C, 2012, 116, 5932-5940.	1.5	83
57	Supramolecular Interactions of Chenodeoxycholic Acid Increase the Efficiency of Dye-Sensitized Solar Cells Based on a Cobalt Electrolyte. Journal of Physical Chemistry C, 2013, 117, 3874-3887.	1.5	82
58	Globularityâ€Selected Large Molecules for a New Generation of Multication Perovskites. Advanced Materials, 2017, 29, 1702005.	11.1	81
59	Inherent electronic trap states in TiO2 nanocrystals: effect of saturation and sintering. Energy and Environmental Science, 2013, 6, 1221.	15.6	76
60	Understanding the Solution Chemistry of Lead Halide Perovskites Precursors. ACS Applied Energy Materials, 2019, 2, 3400-3409.	2.5	74
61	Waterâ€Stable DMASnBr₃ Leadâ€Free Perovskite for Effective Solarâ€Driven Photocatalysis. Angewandte Chemie - International Edition, 2021, 60, 3611-3618.	7.2	72
62	Water Oxidation by the [Co4O4(OAc)4(py)4]+ Cubium is Initiated by OHâ€" Addition. Journal of the American Chemical Society, 2015, 137, 15460-15468.	6.6	64
63	First-Principles Modeling of Bismuth Doping in the MAPbI₃ Perovskite. Journal of Physical Chemistry C, 2018, 122, 14107-14112.	1.5	64
64	Enhanced TiO₂/MAPbI₃ Electronic Coupling by Interface Modification with PbI₂. Chemistry of Materials, 2016, 28, 3612-3615.	3.2	60
65	Long-Lived Photoinduced Polarons in Organohalide Perovskites. Journal of Physical Chemistry Letters, 2017, 8, 3081-3086.	2.1	59
66	Solvent-Free Synthetic Route for Cerium(IV) Metalâ€"Organic Frameworks with UiO-66 Architecture and Their Photocatalytic Applications. ACS Applied Materials & Interfaces, 2019, 11, 45031-45037.	4.0	58
67	Band Gap Engineering in MASnBr₃ and CsSnBr₃ Perovskites: Mechanistic Insights through the Application of Pressure. Journal of Physical Chemistry Letters, 2019, 10, 7398-7405.	2.1	57
68	Surface Reconstruction Engineering with Synergistic Effect of Mixedâ€Salt Passivation Treatment toward Efficient and Stable Perovskite Solar Cells. Advanced Functional Materials, 2021, 31, 2102902.	7.8	57
69	Modeling ZnS and ZnO Nanostructures: Structural, Electronic, and Optical Properties. Journal of Physical Chemistry C, 2011, 115, 25219-25226.	1.5	56
70	Rationalizing the Molecular Design of Holeâ€Selective Contacts to Improve Charge Extraction in Perovskite Solar Cells. Advanced Energy Materials, 2019, 9, 1900990.	10.2	56
71	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.	7.8	53
72	Electronic structure of MAPbI3 and MAPbCl3: importance of band alignment. Scientific Reports, 2019, 9, 15159.	1.6	52

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73	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.	5.2	49
74	Outstanding Passivation Effect by a Mixed-Salt Interlayer with Internal Interactions in Perovskite Solar Cells. ACS Energy Letters, 2020, 5, 3159-3167.	8.8	47
75	Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface. ACS Energy Letters, 2016, 1, 454-463.	8.8	46
76	Energy Level Tuning at the MAPbI₃ Perovskite/Contact Interface Using Chemical Treatment. ACS Energy Letters, 2019, 4, 2181-2184.	8.8	45
77	Charge Localization, Stabilization, and Hopping in Lead Halide Perovskites: Competition between Polaron Stabilization and Cation Disorder. ACS Energy Letters, 2019, 4, 2013-2020.	8.8	43
78	Chlorine Incorporation in the CH₃NH₃PbI₃ Perovskite: Small Concentration, Big Effect. Inorganic Chemistry, 2017, 56, 74-83.	1.9	40
79	New Fullerene Derivative as an nâ€Type Material for Highly Efficient, Flexible Perovskite Solar Cells of a pâ€iâ€n Configuration. Advanced Functional Materials, 2020, 30, 2004357.	7.8	38
80	An Oxa[5]helicene-Based Racemic Semiconducting Glassy Film for Photothermally Stable Perovskite Solar Cells. IScience, 2019, 15, 234-242.	1.9	36
81	Energy vs Charge Transfer in Manganese-Doped Lead Halide Perovskites. ACS Energy Letters, 2021, 6, 1869-1878.	8.8	36
82	Large-scale <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:n -BSE calculations with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>N</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:r scaling: Excitonic effects in dye-sensitized solar cells. Physical Review B, 2017, 95, .	1.1	34
83	First principles modelling of perovskite solar cells based on TiO₂ and Al₂O₃: stability and interfacial electronic structure. Journal of Materials Chemistry A, 2017, 5, 2339-2345.	5.2	34
84	Influence of Disorder and Anharmonic Fluctuations on the Dynamical Rashba Effect in Purely Inorganic Lead-Halide Perovskites. Journal of Physical Chemistry C, 2019, 123, 291-298.	1.5	32
85	Exploring the Limits of Three-Dimensional Perovskites: The Case of FAPb_{1â€"<i>x</i>}Sn_{<i>x</i>}Br₃. ACS Energy Letters, 2018, 3, 1353-1359.	8.8	31
86	Synthesis, Properties, and Modeling of Cs_{1â€"<i>x</i>}Rb<i>_x</i>SnBr₃ Solid Solution: A New Mixed-Cation Lead-Free All-Inorganic Perovskite System. Chemistry of Materials, 2019, 31, 3527-3533.	3.2	30
87	From Experiments to a Fast Easy-to-Use Computational Methodology to Predict Human Aldehyde Oxidase Selectivity and Metabolic Reactions. Journal of Medicinal Chemistry, 2018, 61, 360-371.	2.9	29
88	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.	2.1	29
89	Pyridineâˆ'EDOT Heteroaryleneâˆ'Vinylene Donorâˆ'Acceptor Polymers. Macromolecules, 2010, 43, 9698-9713.	2.2	28
90	Computational modeling of single- versus double-anchoring modes in di-branched organic sensitizers on TiO₂ surfaces: structural and electronic properties. Physical Chemistry Chemical Physics, 2014, 16, 4709-4719.	1.3	28

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91	Computational Modeling of Isoindigo-Based Polymers Used in Organic Solar Cells. Journal of Physical Chemistry C, 2013, 117, 17940-17954.	1.5	27
92	Reaction Mechanism of Photocatalytic Hydrogen Production at Water/Tin Halide Perovskite Interfaces. ACS Energy Letters, 2022, 7, 1308-1315.	8.8	26
93	A vinyleneâ€linked benzo[1,2â€<i>b</i>:4,5â€<i>b'</i>]dithiopheneâ€2,1,3â€benzothiadiazole lowâ€bandgap polymer. Journal of Polymer Science Part A, 2012, 50, 2829-2840.	2.5	25
94	Trends in Perovskite Solar Cells and Optoelectronics: Status of Research and Applications from the PSCO Conference. ACS Energy Letters, 2017, 2, 857-861.	8.8	25
95	Electronic Properties and Carrier Trapping in Bi and Mn Co-doped CsPbCl₃ Perovskite. Journal of Physical Chemistry Letters, 2020, 11, 5482-5489.	2.1	25
96	Transition Dipole Moments of n = 1, 2, and 3 Perovskite Quantum Wells from the Optical Stark Effect and Many-Body Perturbation Theory. Journal of Physical Chemistry Letters, 2020, 11, 716-723.	2.1	24
97	Formation of Color Centers in Lead Iodide Perovskites: Self-Trapping and Defects in the Bulk and Surfaces. Chemistry of Materials, 2020, 32, 6916-6924.	3.2	23
98	A new lead-free 1D hybrid copper perovskite and its structural, thermal, vibrational, optical and magnetic characterization. Journal of Materials Chemistry C, 2021, 9, 5970-5976.	2.7	23
99	A new terpyridine cobalt complex redox shuttle for dye-sensitized solar cells. Inorganica Chimica Acta, 2013, 406, 106-112.	1.2	21
100	Thiocyanateâ€Free Ruthenium(II) Sensitizers for Dyeâ€Sensitized Solar Cells Based on the Cobalt Redox Couple. ChemSusChem, 2014, 7, 2930-2938.	3.6	21
101	Effect of Molecular Fluctuations on Hole Diffusion within Dye Monolayers. Chemistry of Materials, 2014, 26, 4731-4740.	3.2	21
102	Unveiling the nature of post-linear response Z-vector method for time-dependent density functional theory. Journal of Chemical Physics, 2017, 147, 024108.	1.2	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. Journal of Physical Chemistry B, 2020, 124, 11481-11490.	1.2	21
104	Decoding ultrafast polarization responses in lead halide perovskites by the two-dimensional optical Kerr effect. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	21
105	Computational Investigations on Organic Sensitizers for Dye-Sensitized Solar Cell. Current Organic Synthesis, 2012, 9, 215-232.	0.7	20
106	Origin of pressure-induced band gap tuning in tin halide perovskites. Materials Advances, 2020, 1, 2840-2845.	2.6	20
107	Modulating Band Alignment in Mixed Dimensionality 3D/2D Perovskites by Surface Termination Ligand Engineering. Chemistry of Materials, 2020, 32, 105-113.	3.2	19
108	Comparing the excited-state properties of a mixed-cationâ€"mixed-halide perovskite to methylammonium lead iodide. Journal of Chemical Physics, 2020, 152, 104703.	1.2	18

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109	Halide-driven formation of lead halide perovskites: insight from <i>ab initio</i> molecular dynamics simulations. Materials Advances, 2021, 2, 3915-3926.	2.6	18
110	Cation Engineering for Resonant Energy Level Alignment in Two-Dimensional Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 2528-2535.	2.1	17
111	Charge Carriers Are Not Affected by the Relatively Slow-Rotating Methylammonium Cations in Lead Halide Perovskite Thin Films. Journal of Physical Chemistry Letters, 2019, 10, 5128-5134.	2.1	16
112	Structural and Optical Properties of Solvated PbI₂ in Î³-Butyrolactone: Insight into the Solution Chemistry of Lead Halide Perovskite Precursors. Journal of Physical Chemistry Letters, 2020, 11, 6139-6145.	2.1	15
113	Merging of E2 and E1cb Reaction Mechanisms: A Combined Theoretical and Experimental Study. European Journal of Organic Chemistry, 2009, 2009, 5501-5504.	1.2	13
114	Alignment of energy levels in dye/semiconductor interfaces by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m Effects due to coadsorption of solvent molecules. Physical Review B, 2014, 90, .	1.1	13
115	First-Principles Molecular Dynamics in Metal-Halide Perovskites: Contrasting Generalized Gradient Approximation and Hybrid Functionals. Journal of Physical Chemistry Letters, 2021, 12, 11886-11893.	2.1	13
116	Effect of Structural Dynamics on the Opto-Electronic Properties of Bare and Hydrated ZnS QDs. Journal of Physical Chemistry C, 2014, 118, 3274-3284.	1.5	12
117	DFT Investigation of Ligand-Based Reduction of CO₂ to CO on an Anionic Niobium Nitride Complex: Reaction Mechanism and Role of the Na⁺ Counterion. Organometallics, 2011, 30, 4838-4846.	1.1	11
118	Iodide <i>vs</i> Chloride: The Impact of Different Lead Halides on the Solution Chemistry of Perovskite Precursors. ACS Applied Energy Materials, 2021, 4, 9827-9835.	2.5	11
119	Optical and magnetic characterization of one-dimensional Cu(<scp>ii</scp>)-based perovskite: a high UVâ€“Visâ€“NIR absorber. Journal of Materials Chemistry C, 2021, 9, 17158-17166.	2.7	9
120	Boron Functionalization and Unusual Bâ€“C Bond Activation in Rhodium(III) and Iridium(III) Complexes with Diphenylbis(pyrazolylborate) Ligands (Ph₂Bp). Organometallics, 2013, 32, 3895-3902.	1.1	8
121	Dynamical Rashba Band Splitting in Hybrid Perovskites Modeled by Local Electric Fields. Journal of Physical Chemistry C, 2018, 122, 124-132.	1.5	8
122	Designing New Indene-Fullerene Derivatives as Electron-Transporting Materials for Flexible Perovskite Solar Cells. Journal of Physical Chemistry C, 2021, 125, 27344-27353.	1.5	8
123	Thermal Fluctuations on FÃ¶rster Resonance Energy Transfer in Dyadic Solar Cell Sensitizers: A Combined Ab Initio Molecular Dynamics and TDDFT Investigation. Journal of Physical Chemistry C, 2015, 119, 16490-16499.	1.5	6
124	Zn2+ and Cu2+ doping of one-dimensional lead-free hybrid perovskite ABX3 for white light emission and green solar cell applications. Materials Research Bulletin, 2022, 151, 111819.	2.7	6
125	A DFT investigation of base-catalyzed Î²-elimination reactions in water solution for systems activated by the pyridine ring: Theory vs. experiment. Chemical Physics Letters, 2008, 460, 100-107.	1.2	5
126	DFT studies of Î²-elimination reactions in water solution with different bases: Theory vs experiment. Computational and Theoretical Chemistry, 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.	2.1	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.	0.2	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