

Edoardo Mosconi

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

132
papers

18,686
citations

57
h-index

136
g-index

138
ext. papers

21,214
ext. citations

12
avg, IF

7.15
L-index

#	Paper	IF	Citations
132	Understanding Performance Limiting Interfacial Recombination in pin Perovskite Solar Cells. <i>Advanced Energy Materials</i> , 2022 , 2103567	21.8	13
131	Reaction Mechanism of Photocatalytic Hydrogen Production at Water/Tin Halide Perovskite Interfaces. <i>ACS Energy Letters</i> , 2022 , 7, 1308-1315	20.1	5
130	Stability of Tin- versus Lead-Halide Perovskites: Ab Initio Molecular Dynamics Simulations of Perovskite/Water Interfaces.. <i>Journal of Physical Chemistry Letters</i> , 2022 , 2321-2329	6.4	7
129	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	5.1	0
128	First-Principles Molecular Dynamics in Metal-Halide Perovskites: Contrasting Generalized Gradient Approximation and Hybrid Functionals. <i>Journal of Physical Chemistry Letters</i> , 2021 , 11886-11893	6.4	4
127	Tuning structural isomers of phenylenediammonium to afford efficient and stable perovskite solar cells and modules. <i>Nature Communications</i> , 2021 , 12, 6394	17.4	23
126	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	3.8	4
125	Optical and magnetic characterization of one-dimensional Cu(II)-based perovskite: a high UV-Vis-NIR absorber. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 17158-17166	7.1	3
124	Ligand-engineered bandgap stability in mixed-halide perovskite LEDs. <i>Nature</i> , 2021 , 591, 72-77	50.4	172
123	Cation Engineering for Resonant Energy Level Alignment in Two-Dimensional Lead Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 2528-2535	6.4	4
122	Energy vs Charge Transfer in Manganese-Doped Lead Halide Perovskites.. <i>ACS Energy Letters</i> , 2021 , 6, 1869-1878	20.1	12
121	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	15.6	17
120	Real Space-Real Time Evolution of Excitonic States Based on the Bethe-Salpeter Equation Method. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 7261-7269	6.4	2
119	Water-Stable DMASnBr Lead-Free Perovskite for Effective Solar-Driven Photocatalysis. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 3611-3618	16.4	29
118	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	7.1	11
117	Halide-driven formation of lead halide perovskites: insight from ab initio molecular dynamics simulations. <i>Materials Advances</i> , 2021 , 2, 3915-3926	3.3	5
116	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,	11.5	8

115	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	6.1	2
114	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 , 2104428	15.6	14
113	Electronic Properties and Carrier Trapping in Bi and Mn Co-doped CsPbCl Perovskite. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5482-5489	6.4	14
112	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	13	28
111	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	3.9	8
110	Structural and Optical Properties of Solvated Pbl in ϵ -Butyrolactone: Insight into the Solution Chemistry of Lead Halide Perovskite Precursors. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 6139-6145	6.4	10
109	Transition Dipole Moments of = 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	6.4	14
108	The Doping Mechanism of Halide Perovskite Unveiled by Alkaline Earth Metals. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2364-2374	16.4	65
107	Modulating Band Alignment in Mixed Dimensionality 3D/2D Perovskites by Surface Termination Ligand Engineering. <i>Chemistry of Materials</i> , 2020 , 32, 105-113	9.6	12
106	Polarons in Metal Halide Perovskites. <i>Advanced Energy Materials</i> , 2020 , 10, 1902748	21.8	47
105	Origin of pressure-induced band gap tuning in tin halide perovskites. <i>Materials Advances</i> , 2020 , 1, 2840-2845	3.4	10
104	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	9.6	15
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	3.4	12
102	Outstanding Passivation Effect by a Mixed-Salt Interlayer with Internal Interactions in Perovskite Solar Cells. <i>ACS Energy Letters</i> , 2020 , 5, 3159-3167	20.1	22
101	New Fullerene Derivative as an n-Type Material for Highly Efficient, Flexible Perovskite Solar Cells of a p-i-n Configuration. <i>Advanced Functional Materials</i> , 2020 , 30, 2004357	15.6	25
100	Controlling competing photochemical reactions stabilizes perovskite solar cells. <i>Nature Photonics</i> , 2019 , 13, 532-539	33.9	161
99	Rationalizing the Molecular Design of Hole-Selective Contacts to Improve Charge Extraction in Perovskite Solar Cells. <i>Advanced Energy Materials</i> , 2019 , 9, 1900990	21.8	37
98	An Oxa[5]helicene-Based Racemic Semiconducting Glassy Film for Photothermally Stable Perovskite Solar Cells. <i>iScience</i> , 2019 , 15, 234-242	6.1	24

97	Understanding the Solution Chemistry of Lead Halide Perovskites Precursors. <i>ACS Applied Energy Materials</i> , 2019 , 2, 3400-3409	6.1	40
96	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	9.6	21
95	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	6.4	11
94	Energy Level Tuning at the MAPbI ₃ Perovskite/Contact Interface Using Chemical Treatment. <i>ACS Energy Letters</i> , 2019 , 4, 2181-2184	20.1	31
93	Stabilizing halide perovskite surfaces for solar cell operation with wide-bandgap lead oxysalts. <i>Science</i> , 2019 , 365, 473-478	33.3	460
92	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	20.1	32
91	Electronic structure of MAPbI and MAPbCl: importance of band alignment. <i>Scientific Reports</i> , 2019 , 9, 15159	4.9	21
90	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	9.5	34
89	Band Gap Engineering in MASnBr and CsSnBr Perovskites: Mechanistic Insights through the Application of Pressure. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 7398-7405	6.4	31
88	Formation of Surface Defects Dominates Ion Migration in Lead-Halide Perovskites. <i>ACS Energy Letters</i> , 2019 , 4, 779-785	20.1	135
87	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	3.8	21
86	Infrared Dielectric Screening Determines the Low Exciton Binding Energy of Metal-Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 620-627	6.4	62
85	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	20.1	66
84	Iodine chemistry determines the defect tolerance of lead-halide perovskites. <i>Energy and Environmental Science</i> , 2018 , 11, 702-713	35.4	353
83	First-Principles Modeling of Bismuth Doping in the MAPbI ₃ Perovskite. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 14107-14112	3.8	41
82	Ultrafast THz Fingerprints of Large Polaron formation in Lead-Halide Perovskites 2018 ,		1
81	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	8.3	21
80	Dynamical Rashba Band Splitting in Hybrid Perovskites Modeled by Local Electric Fields. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 124-132	3.8	7

79	Large electrostrictive response in lead halide perovskites. <i>Nature Materials</i> , 2018 , 17, 1020-1026	27	89
78	Ionotronic Halide Perovskite Drift-Diffusive Synapses for Low-Power Neuromorphic Computation. <i>Advanced Materials</i> , 2018 , 30, e1805454	24	91
77	Exploring the Limits of Three-Dimensional Perovskites: The Case of FAPb _{1-x} Sn _x Br ₃ . <i>ACS Energy Letters</i> , 2018 , 3, 1353-1359	20.1	23
76	Nearly Monodisperse Insulator CsPbX (X = Cl, Br, I) Nanocrystals, Their Mixed Halide Compositions, and Their Transformation into CsPbX Nanocrystals. <i>Nano Letters</i> , 2017 , 17, 1924-1930	11.5	378
75	Defect-Assisted Photoinduced Halide Segregation in Mixed-Halide Perovskite Thin Films. <i>ACS Energy Letters</i> , 2017 , 2, 1416-1424	20.1	307
74	Rashba Band Splitting in Organohalide Lead Perovskites: Bulk and Surface Effects. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2247-2252	6.4	76
73	Long-Lived Photoinduced Polarons in Organohalide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 3081-3086	6.4	45
72	One-Year stable perovskite solar cells by 2D/3D interface engineering. <i>Nature Communications</i> , 2017 , 8, 15684	17.4	1253
71	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	20.1	21
70	Large-scale GW-BSE calculations with N ³ scaling: Excitonic effects in dye-sensitized solar cells. <i>Physical Review B</i> , 2017 , 95,	3.3	22
69	Broadband Emission in Two-Dimensional Hybrid Perovskites: The Role of Structural Deformation. <i>Journal of the American Chemical Society</i> , 2017 , 139, 39-42	16.4	253
68	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	13	28
67	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	3.9	21
66	Globularity-Selected Large Molecules for a New Generation of Multication Perovskites. <i>Advanced Materials</i> , 2017 , 29, 1702005	24	67
65	Large polarons in lead halide perovskites. <i>Science Advances</i> , 2017 , 3, e1701217	14.3	374
64	Mechanism of Reversible Trap Passivation by Molecular Oxygen in Lead-Halide Perovskites. <i>ACS Energy Letters</i> , 2017 , 2, 2794-2798	20.1	86
63	Chlorine Incorporation in the CH ₃ NH ₃ PbI Perovskite: Small Concentration, Big Effect. <i>Inorganic Chemistry</i> , 2017 , 56, 74-83	5.1	36
62	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	13.4	355

61	Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface. <i>ACS Energy Letters</i> , 2016 , 1, 454-463	20.1	39
60	Light-induced annihilation of Frenkel defects in organo-lead halide perovskites. <i>Energy and Environmental Science</i> , 2016 , 9, 3180-3187	35.4	243
59	A molecularly engineered hole-transporting material for efficient perovskite solar cells. <i>Nature Energy</i> , 2016 , 1,	62.3	693
58	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, 1010-6	16.4	615
57	Chapter 8:First Principles Modeling of Perovskite Solar Cells: Interplay of Structural, Electronic and Dynamical Effects. <i>RSC Energy and Environment Series</i> , 2016 , 234-296	0.6	2
56	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	16.4	141
55	Enhanced TiO ₂ /MAPbI ₃ Electronic Coupling by Interface Modification with PbI ₂ . <i>Chemistry of Materials</i> , 2016 , 28, 3612-3615	9.6	54
54	Mobile Ions in Organohalide Perovskites: Interplay of Electronic Structure and Dynamics. <i>ACS Energy Letters</i> , 2016 , 1, 182-188	20.1	143
53	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, 1638-45	6.4	220
52	High Open-Circuit Voltage: Fabrication of Formamidinium Lead Bromide Perovskite Solar Cells Using FluoreneDithiophene Derivatives as Hole-Transporting Materials. <i>ACS Energy Letters</i> , 2016 , 1, 107-112	20.1	92
51	Electronic and optical properties of MAPbX perovskites (X = I, Br, Cl): a unified DFT and GW theoretical analysis. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 27158-27164	3.6	108
50	First-Principles Modeling of Organohalide Thin Films and Interfaces 2016 , 19-52		4
49	Structural and electronic properties of organo-halide hybrid perovskites from ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 9394-409	3.6	116
48	Ab Initio Molecular Dynamics Simulations of Methylammonium Lead Iodide Perovskite Degradation by Water. <i>Chemistry of Materials</i> , 2015 , 27, 4885-4892	9.6	323
47	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	3.8	6
46	Intrinsic Thermal Instability of Methylammonium Lead Trihalide Perovskite. <i>Advanced Energy Materials</i> , 2015 , 5, 1500477	21.8	1386
45	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	9.4	171
44	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, 15460-8	16.4	58

43	Photoinduced Reversible Structural Transformations in Free-Standing CH ₃ NH ₃ PbI ₃ Perovskite Films. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 2332-8	6.4	172
42	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	9.6	448
41	Defect migration in methylammonium lead iodide and its role in perovskite solar cell operation. <i>Energy and Environmental Science</i> , 2015 , 8, 2118-2127	35.4	1003
40	Electronic and optical properties of mixed SnPb organohalide perovskites: a first principles investigation. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 9208-9215	13	156
39	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	4.9	910
38	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	3.8	11
37	Stark effect in perovskite/TiO ₂ solar cells: evidence of local interfacial order. <i>Nano Letters</i> , 2014 , 14, 2168-74	11.5	182
36	Cation-induced band-gap tuning in organohalide perovskites: interplay of spin-orbit coupling and octahedra tilting. <i>Nano Letters</i> , 2014 , 14, 3608-16	11.5	837
35	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, 279-84	6.4	476
34	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, 4709-19	3.6	26
33	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	9.6	252
32	First-Principles Investigation of the TiO ₂ /Organohalide Perovskites Interface: The Role of Interfacial Chlorine. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 2619-25	6.4	228
31	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, 2662-9	6.4	277
30	Elusive Presence of Chloride in Mixed Halide Perovskite Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3532-8	6.4	160
29	Thiocyanate-free ruthenium(II) sensitizers for dye-sensitized solar cells based on the cobalt redox couple. <i>ChemSusChem</i> , 2014 , 7, 2930-8	8.3	18
28	Effect of Molecular Fluctuations on Hole Diffusion within Dye Monolayers. <i>Chemistry of Materials</i> , 2014 , 26, 4731-4740	9.6	20
27	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, 16137-44	3.6	195
26	MAPbI ₃ -xCl _x mixed halide perovskite for hybrid solar cells: the role of chloride as dopant on the transport and structural properties. <i>Materials Research Society Symposia Proceedings</i> , 2014 , 1667, 41		2

25	Alignment of energy levels in dye/semiconductor interfaces by GW calculations: Effects due to coadsorption of solvent molecules. <i>Physical Review B</i> , 2014 , 90,	3.3	11
24	Investigating Charge Dynamics in Halide Perovskite Sensitized Mesoporous Solar Cells. <i>Materials Research Society Symposia Proceedings</i> , 2014 , 1667, 7		2
23	A new terpyridine cobalt complex redox shuttle for dye-sensitized solar cells. <i>Inorganica Chimica Acta</i> , 2013 , 406, 106-112	2.7	18
22	Boron Functionalization and Unusual B-C Bond Activation in Rhodium(III) and Iridium(III) Complexes with Diphenylbis(pyrazolylborate) Ligands (Ph ₂ Bp). <i>Organometallics</i> , 2013 , 32, 3895-3902	3.8	7
21	Computational Modeling of Isoindigo-Based Polymers Used in Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 17940-17954	3.8	27
20	MAPbI ₃ -xCl _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	9.6	658
19	Inherent electronic trap states in TiO ₂ nanocrystals: effect of saturation and sintering. <i>Energy and Environmental Science</i> , 2013 , 6, 1221	35.4	68
18	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	3.8	76
17	First-Principles Modeling of Mixed Halide Organometal Perovskites for Photovoltaic Applications. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 13902-13913	3.8	767
16	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, 19438-53	16.4	185
15	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, 15963-74	3.6	133
14	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	2.5	20
13	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	3.8	74
12	Computational Investigation of Dye/Dye Interactions in Organic Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 5965-5973	3.8	82
11	Computational Investigations on Organic Sensitizers for Dye-Sensitized Solar Cell. <i>Current Organic Synthesis</i> , 2012 , 9, 215-232	1.9	18
10	Modeling ZnS and ZnO Nanostructures: Structural, Electronic, and Optical Properties. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 25219-25226	3.8	51
9	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	3.8	200
8	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	3.8	10

7	Pyridine- π -DOT Heteroarylene-Vinylene Donor-Acceptor Polymers?. <i>Macromolecules</i> , 2010 , 43, 9698-9713	5.5	22
6	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	3.8	302
5	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		3
4	Merging of E2 and E1cb Reaction Mechanisms: A Combined Theoretical and Experimental Study. <i>European Journal of Organic Chemistry</i> , 2009 , 2009, 5501-5504	3.2	10
3	Di-branched di-anchoring organic dyes for dye-sensitized solar cells. <i>Energy and Environmental Science</i> , 2009 , 2, 1094	35.4	175
2	High open-circuit voltage solid-state dye-sensitized solar cells with organic dye. <i>Nano Letters</i> , 2009 , 9, 2487-92	11.5	220
1	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	2.5	5