Filippo De Angelis

List of Publications by Year in Descending Order

373 papers	34,791 citations	89 h-index	178 g-index
389 ext. papers	38,449 ext. citations	10.3 avg, IF	7.7 L-index

#	Paper	IF	Citations
373	Role of the Alkali Metal Cation in the Early Stages of Crystallization of Halide Perovskites. *Chemistry of Materials*, **2022**, 34, 1121-1131	9.6	2
372	Understanding Performance Limiting Interfacial Recombination in pin Perovskite Solar Cells. *Advanced Energy Materials*, **2022**, 2103567	21.8	13
371	Reaction Mechanism of Photocatalytic Hydrogen Production at Water/Tin Halide Perovskite Interfaces. *ACS Energy Letters*, **2022**, 7, 1308-1315	20.1	5
370	Stability of Tin- versus Lead-Halide Perovskites: Ab Initio Molecular Dynamics Simulations of Perovskite/Water Interfaces.. *Journal of Physical Chemistry Letters*, **2022**, 2321-2329	6.4	7
369	Single-crystalline TiO nanoparticles for stable and efficient perovskite modules.. *Nature Nanotechnology*, **2022**,	28.7	13
368	Modelling the Interaction between Carboxylic Acids and Zinc Oxide: Insight into Degradation of ZnO Pigments. *Molecules*, **2022**, 27, 3362	4.8	0
367	First-Principles Molecular Dynamics in Metal-Halide Perovskites: Contrasting Generalized Gradient Approximation and Hybrid Functionals. *Journal of Physical Chemistry Letters*, **2021**, 11886-11893	6.4	4
366	Tuning structural isomers of phenylenediammonium to afford efficient and stable perovskite solar cells and modules. *Nature Communications*, **2021**, 12, 6394	17.4	23
365	Designing New Indene-Fullerene Derivatives as Electron-Transporting Materials for Flexible Perovskite Solar Cells.. *Journal of Physical Chemistry C*, **2021**, 125, 27344-27353	3.8	4
364	The Prospect of Lead-Free Perovskite Photovoltaics. *ACS Energy Letters*, **2021**, 6, 1586-1587	20.1	13
363	Ligand-engineered bandgap stability in mixed-halide perovskite LEDs. *Nature*, **2021**, 591, 72-77	50.4	172
362	Cation Engineering for Resonant Energy Level Alignment in Two-Dimensional Lead Halide Perovskites. *Journal of Physical Chemistry Letters*, **2021**, 12, 2528-2535	6.4	4
361	Energy vs Charge Transfer in Manganese-Doped Lead Halide Perovskites.. *ACS Energy Letters*, **2021**, 6, 1869-1878	20.1	12
360	Suppression of Tin Oxidation by 3D/2D Perovskite Interfacing. *Journal of Physical Chemistry C*, **2021**, 125, 10901-10908	3.8	4
359	Surface Reconstruction Engineering with Synergistic Effect of Mixed-Salt Passivation Treatment toward Efficient and Stable Perovskite Solar Cells. *Advanced Functional Materials*, **2021**, 31, 2102902	15.6	17
358	Energy Spotlight. *ACS Energy Letters*, **2021**, 6, 2635-2637	20.1	
357	Observation of large Rashba spin□rbit coupling at room temperature in compositionally engineered perovskite single crystals and application in high performance photodetectors. *Materials Today*, **2021**, 46, 18-27	21.8	9

356	Strong Electron Localization in Tin Halide Perovskites. *Journal of Physical Chemistry Letters*, **2021**, 12, 5339-5343	6.4	9
355	Multication perovskite 2D/3D interfaces form via progressive dimensional reduction. *Nature Communications*, **2021**, 12, 3472	17.4	24
354	Real Space-Real Time Evolution of Excitonic States Based on the Bethe-Salpeter Equation Method. *Journal of Physical Chemistry Letters*, **2021**, 12, 7261-7269	6.4	2
353	Water-Stable DMASnBr Lead-Free Perovskite for Effective Solar-Driven Photocatalysis. *Angewandte Chemie - International Edition*, **2021**, 60, 3611-3618	16.4	29
352	Tuning halide perovskite energy levels. *Energy and Environmental Science*, **2021**, 14, 1429-1438	35.4	38
351	Water-Stable DMASnBr3 Lead-Free Perovskite for Effective Solar-Driven Photocatalysis. *Angewandte Chemie*, **2021**, 133, 3655-3662	3.6	2
350	The dependence of the spectroscopic properties of orcein dyes on solvent proticity: insights from theory and experiments. *Physical Chemistry Chemical Physics*, **2021**, 23, 15329-15337	3.6	
349	Halide-driven formation of lead halide perovskites: insight from ab initio molecular dynamics simulations. *Materials Advances*, **2021**, 2, 3915-3926	3.3	5
348	Combination of a large cation and coordinating additive improves carrier transport properties in quasi-2D perovskite solar cells. *Journal of Materials Chemistry A*, **2021**, 9, 9175-9190	13	2
347	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,	11.5	8
346	Composition-Dependent Struggle between Iodine and Tin Chemistry at the Surface of Mixed Tin/Lead Perovskites. *ACS Energy Letters*, **2021**, 6, 969-976	20.1	12
345	Solvents for Processing Stable Tin Halide Perovskites. *ACS Energy Letters*, **2021**, 6, 959-968	20.1	35
344	Halogen-Bonded Hole-Transport Material Suppresses Charge Recombination and Enhances Stability of Perovskite Solar Cells. *Advanced Energy Materials*, **2021**, 11, 2101553	21.8	13
343	Iodide vs Chloride: The Impact of Different Lead Halides on the Solution Chemistry of Perovskite Precursors. *ACS Applied Energy Materials*, **2021**, 4, 9827-9835	6.1	2
342	Experimental Strategy and Mechanistic View to Boost the Photocatalytic Activity of Cs3Bi2Br9 Lead-Free Perovskite Derivative by g-C3N4 Composite Engineering. *Advanced Functional Materials*, **2021**, 2104428	15.6	14
341	Role of spacer cations and structural distortion in two-dimensional germanium halide perovskites. *Journal of Materials Chemistry C*, **2021**, 9, 9899-9906	7.1	6
340	Electronic Properties and Carrier Trapping in Bi and Mn Co-doped CsPbCl Perovskite. *Journal of Physical Chemistry Letters*, **2020**, 11, 5482-5489	6.4	14
339	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	13	28

338	Evolution of Perovskite Solar Cells: Lessons Learned from Hybrid/Organic Photovoltaics. *ACS Energy Letters*, **2020**, 5, 935-937	20.1	0
337	Structural and Optical Properties of Solvated PbI in Butyrolactone: Insight into the Solution Chemistry of Lead Halide Perovskite Precursors. *Journal of Physical Chemistry Letters*, **2020**, 11, 6139-6145	6.4	10
336	Transition Dipole Moments of = 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	6.4	14
335	Tin versus Lead Redox Chemistry Modulates Charge Trapping and Self-Doping in Tin/Lead Iodide Perovskites. *Journal of Physical Chemistry Letters*, **2020**, 11, 3546-3556	6.4	64
334	The Doping Mechanism of Halide Perovskite Unveiled by Alkaline Earth Metals. *Journal of the American Chemical Society*, **2020**, 142, 2364-2374	16.4	65
333	Modulating Band Alignment in Mixed Dimensionality 3D/2D Perovskites by Surface Termination Ligand Engineering. *Chemistry of Materials*, **2020**, 32, 105-113	9.6	12
332	Polarons in Metal Halide Perovskites. *Advanced Energy Materials*, **2020**, 10, 1902748	21.8	47
331	Origin of pressure-induced band gap tuning in tin halide perovskites. *Materials Advances*, **2020**, 1, 2840-2845	3.4	10
330	Formation of Color Centers in Lead Iodide Perovskites: Self-Trapping and Defects in the Bulk and Surfaces. *Chemistry of Materials*, **2020**, 32, 6916-6924	9.6	15
329	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	3.4	12
328	Universal approach toward high-efficiency two-dimensional perovskite solar cells via a vertical-rotation process. *Energy and Environmental Science*, **2020**, 13, 3093-3101	35.4	46
327	Instability of Tin Iodide Perovskites: Bulk p-Doping versus Surface Tin Oxidation. *ACS Energy Letters*, **2020**, 5, 2787-2795	20.1	67
326	Critical Role of Protons for Emission Quenching of Indoline Dyes in Solution and on Semiconductor Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 21346-21356	3.8	6
325	Outstanding Passivation Effect by a Mixed-Salt Interlayer with Internal Interactions in Perovskite Solar Cells. *ACS Energy Letters*, **2020**, 5, 3159-3167	20.1	22
324	New Fullerene Derivative as an n-Type Material for Highly Efficient, Flexible Perovskite Solar Cells of a p-i-n Configuration. *Advanced Functional Materials*, **2020**, 30, 2004357	15.6	25
323	A combined experimental and theoretical approach revealing a direct mechanism for bifunctional water splitting on doped copper phosphide. *Nanoscale*, **2020**, 12, 17769-17779	7.7	5
322	Ab Initio Modeling of Solar Cell Dye Sensitizers: The Hunt for Red Photons Continues. *European Journal of Inorganic Chemistry*, **2019**, 2019, 743-750	2.3	5
321	Controlling competing photochemical reactions stabilizes perovskite solar cells. *Nature Photonics*, **2019**, 13, 532-539	33.9	161

320	Stable Ligand Coordination at the Surface of Colloidal CsPbBr Nanocrystals. *Journal of Physical Chemistry Letters*, **2019**, 10, 3715-3726	6.4	49
319	Electrochemical Hole Injection Selectively Expels Iodide from Mixed Halide Perovskite Films. *Journal of the American Chemical Society*, **2019**, 141, 10812-10820	16.4	73
318	Rationalizing the Molecular Design of Hole-Selective Contacts to Improve Charge Extraction in Perovskite Solar Cells. *Advanced Energy Materials*, **2019**, 9, 1900990	21.8	37
317	Mo6S3Br6: An Anisotropic 2D Superatomic Semiconductor. *Advanced Functional Materials*, **2019**, 29, 1902951	15.6	6
316	Interface Electrostatics of Solid-State Dye-Sensitized Solar Cells: A Joint Drift-Diffusion and Density Functional Theory Study. *Journal of Physical Chemistry C*, **2019**, 123, 14955-14963	3.8	5
315	Large polaron evidence in the ultrafast THz response of Lead-Halide Perovskites. *EPJ Web of Conferences*, **2019**, 205, 04019	0.3	
314	An Oxa[5]helicene-Based Racemic Semiconducting Glassy Film for Photothermally Stable Perovskite Solar Cells. *IScience*, **2019**, 15, 234-242	6.1	24
313	Ultrafast THz Probe of Photoinduced Polarons in Lead-Halide Perovskites. *Physical Review Letters*, **2019**, 122, 166601	7.4	56
312	Understanding the Solution Chemistry of Lead Halide Perovskites Precursors. *ACS Applied Energy Materials*, **2019**, 2, 3400-3409	6.1	40
311	Synthesis, Properties, and Modeling of Cs1−xRbxSnBr3 Solid Solution: A New Mixed-Cation Lead-Free All-Inorganic Perovskite System. *Chemistry of Materials*, **2019**, 31, 3527-3533	9.6	21
310	From Large to Small Polarons in Lead, Tin, and Mixed Lead-Tin Halide Perovskites. *Journal of Physical Chemistry Letters*, **2019**, 10, 1790-1798	6.4	49
309	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	6.4	11
308	Energy Level Tuning at the MAPbI3 Perovskite/Contact Interface Using Chemical Treatment. *ACS Energy Letters*, **2019**, 4, 2181-2184	20.1	31
307	Defect Activity in Lead Halide Perovskites. *Advanced Materials*, **2019**, 31, e1901183	24	119
306	Ligand-Induced Surface Charge Density Modulation Generates Local Type-II Band Alignment in Reduced-Dimensional Perovskites. *Journal of the American Chemical Society*, **2019**, 141, 13459-13467	16.4	41
305	Stabilizing halide perovskite surfaces for solar cell operation with wide-bandgap lead oxysalts. *Science*, **2019**, 365, 473-478	33.3	460
304	Hierarchical Coherent Phonons in a Superatomic Semiconductor. *Advanced Materials*, **2019**, 31, e1903209	24	5
303	Charge Localization, Stabilization, and Hopping in Lead Halide Perovskites: Competition between Polaron Stabilization and Cation Disorder. *ACS Energy Letters*, **2019**, 4, 2013-2020	20.1	32

302	The nature of the lead-iodine bond in PbI2: A case study for the modelling of lead halide perovskites. *Computational and Theoretical Chemistry*, **2019**, 1164, 112558	2	6
301	Electronic structure of MAPbI and MAPbCl: importance of band alignment. *Scientific Reports*, **2019**, 9, 15159	4.9	21
300	Solvent-Free Synthetic Route for Cerium(IV) Metal-Organic Frameworks with UiO-66 Architecture and Their Photocatalytic Applications. *ACS Applied Materials & Interfaces*, **2019**, 11, 45031-45037	9.5	34
299	Introduction of a Bifunctional Cation Affords Perovskite Solar Cells Stable at Temperatures Exceeding 80 °C. *ACS Energy Letters*, **2019**, 4, 2989-2994	20.1	13
298	Band Gap Engineering in MASnBr and CsSnBr Perovskites: Mechanistic Insights through the Application of Pressure. *Journal of Physical Chemistry Letters*, **2019**, 10, 7398-7405	6.4	31
297	Formation of Surface Defects Dominates Ion Migration in Lead-Halide Perovskites. *ACS Energy Letters*, **2019**, 4, 779-785	20.1	135
296	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	3.8	21
295	Clues from defect photochemistry. *Nature Materials*, **2018**, 17, 383-384	27	28
294	Infrared Dielectric Screening Determines the Low Exciton Binding Energy of Metal-Halide Perovskites. *Journal of Physical Chemistry Letters*, **2018**, 9, 620-627	6.4	62
293	Modeling the Interaction of Molecular Iodine with MAPbI3: A Probe of Lead-Halide Perovskites Defect Chemistry. *ACS Energy Letters*, **2018**, 3, 447-451	20.1	66
292	Iodine chemistry determines the defect tolerance of lead-halide perovskites. *Energy and Environmental Science*, **2018**, 11, 702-713	35.4	353
291	Superatomic Two-Dimensional Semiconductor. *Nano Letters*, **2018**, 18, 1483-1488	11.5	25
290	Origin of low electron□hole recombination rate in metal halide perovskites. *Energy and Environmental Science*, **2018**, 11, 101-105	35.4	86
289	First-Principles Modeling of Bismuth Doping in the MAPbI3 Perovskite. *Journal of Physical Chemistry C*, **2018**, 122, 14107-14112	3.8	41
288	Light-Induced Formation of Pb3+ Paramagnetic Species in Lead Halide Perovskites. *ACS Energy Letters*, **2018**, 3, 1840-1847	20.1	20
287	First-Principles Modeling of Defects in Lead Halide Perovskites: Best Practices and Open Issues. *ACS Energy Letters*, **2018**, 3, 2206-2222	20.1	152
286	Dye-Sensitized Photocatalytic Hydrogen Generation: Efficiency Enhancement by Organic Photosensitizer□oadsorbent Intermolecular Interaction. *ACS Energy Letters*, **2018**, 3, 85-91	20.1	39
285	Dynamical Rashba Band Splitting in Hybrid Perovskites Modeled by Local Electric Fields. *Journal of Physical Chemistry C*, **2018**, 122, 124-132	3.8	7

284	Quantitative structure-property relationship modeling of small organic molecules for solar cells applications. *Journal of Chemometrics*, **2018**, 32, e2957	1.6	5
283	Large electrostrictive response in lead halide perovskites. *Nature Materials*, **2018**, 17, 1020-1026	27	89
282	Ionotronic Halide Perovskite Drift-Diffusive Synapses for Low-Power Neuromorphic Computation. *Advanced Materials*, **2018**, 30, e1805454	24	91
281	Exploring the Limits of Three-Dimensional Perovskites: The Case of FAPb1⊠SnxBr3. *ACS Energy Letters*, **2018**, 3, 1353-1359	20.1	23
280	Influence of Surface Termination on the Energy Level Alignment at the CH3NH3PbI3 Perovskite/C60 Interface. *Chemistry of Materials*, **2017**, 29, 958-968	9.6	119
279	Migration of cations induces reversible performance losses over day/night cycling in perovskite solar cells. *Energy and Environmental Science*, **2017**, 10, 604-613	35.4	387
278	Nearly Monodisperse Insulator CsPbX (X = Cl, Br, I) Nanocrystals, Their Mixed Halide Compositions, and Their Transformation into CsPbX Nanocrystals. *Nano Letters*, **2017**, 17, 1924-1930	11.5	378
277	Riding the New Wave of Perovskites. *ACS Energy Letters*, **2017**, 2, 922-923	20.1	13
276	Defect-Assisted Photoinduced Halide Segregation in Mixed-Halide Perovskite Thin Films. *ACS Energy Letters*, **2017**, 2, 1416-1424	20.1	307
275	A ruthenium tetrazole complex-based high efficiency near infrared light electrochemical cell. *Chemical Communications*, **2017**, 53, 6211-6214	5.8	12
274	Rashba Band Splitting in Organohalide Lead Perovskites: Bulk and Surface Effects. *Journal of Physical Chemistry Letters*, **2017**, 8, 2247-2252	6.4	76
273	Long-Lived Photoinduced Polarons in Organohalide Perovskites. *Journal of Physical Chemistry Letters*, **2017**, 8, 3081-3086	6.4	45
272	Trends in Perovskite Solar Cells and Optoelectronics: Status of Research and Applications from the PSCO Conference. *ACS Energy Letters*, **2017**, 2, 857-861	20.1	21
271	Large-scale GW-BSE calculations with N3 scaling: Excitonic effects in dye-sensitized solar cells. *Physical Review B*, **2017**, 95,	3.3	22
270	Broadband Emission in Two-Dimensional Hybrid Perovskites: The Role of Structural Deformation. *Journal of the American Chemical Society*, **2017**, 139, 39-42	16.4	253
269	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	13	28
268	A Conversation with Henry Snaith. *ACS Energy Letters*, **2017**, 2, 2552-2554	20.1	1
267	Fluorescent Alloy CsPb Mn I Perovskite Nanocrystals with High Structural and Optical Stability. *ACS Energy Letters*, **2017**, 2, 2183-2186	20.1	224

266	Globularity-Selected Large Molecules for a New Generation of Multication Perovskites. *Advanced Materials*, **2017**, 29, 1702005	24	67
265	Large polarons in lead halide perovskites. *Science Advances*, **2017**, 3, e1701217	14.3	374
264	Mechanism of Reversible Trap Passivation by Molecular Oxygen in Lead-Halide Perovskites. *ACS Energy Letters*, **2017**, 2, 2794-2798	20.1	86
263	Perovskite Solar Cells on Their Way to the Market. *ACS Energy Letters*, **2017**, 2, 2640-2641	20.1	5
262	A Conversation with Michael Grätzel. *ACS Energy Letters*, **2017**, 2, 1674-1676	20.1	11
261	Chlorine Incorporation in the CHNHPbI Perovskite: Small Concentration, Big Effect. *Inorganic Chemistry*, **2017**, 56, 74-83	5.1	36
260	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	35.4	355
259	Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface. *ACS Energy Letters*, **2016**, 1, 454-463	20.1	39
258	Cobalt Polypyridyl Complexes as Transparent Solution-Processable Solid-State Charge Transport Materials. *Advanced Energy Materials*, **2016**, 6, 1600874	21.8	17
257	Ab Initio Simulation of the Absorption Spectra of Photoexcited Carriers in TiO2 Nanoparticles. *Journal of Physical Chemistry Letters*, **2016**, 7, 3597-602	6.4	20
256	Light-induced annihilation of Frenkel defects in organo-lead halide perovskites. *Energy and Environmental Science*, **2016**, 9, 3180-3187	35.4	243
255	A molecularly engineered hole-transporting material for efficient perovskite solar cells. *Nature Energy*, **2016**, 1,	62.3	693
254	Ligand Engineering for the Efficient Dye-Sensitized Solar Cells with Ruthenium Sensitizers and Cobalt Electrolytes. *Inorganic Chemistry*, **2016**, 55, 6653-9	5.1	65
253	Benchmarking DFT and semi-empirical methods for a reliable and cost-efficient computational screening of benzofulvene derivatives as donor materials for small-molecule organic solar cells. *Journal of Physics Condensed Matter*, **2016**, 28, 074005	1.8	27
252	Theoretical Investigation of Adsorption, Dynamics, Self-Aggregation, and Spectroscopic Properties of the D102 Indoline Dye on an Anatase (101) Substrate. *Journal of Physical Chemistry C*, **2016**, 120, 2787-2796	3.8	20
251	New terpyridine-based ruthenium complexes for dye sensitized solar cells applications. *Inorganica Chimica Acta*, **2016**, 442, 158-166	2.7	16
250	Structural and electronic properties of dye-sensitized TiO2 for solar cell applications: from single molecules to self-assembled monolayers. *Journal of Materials Chemistry C*, **2016**, 4, 4346-4373	7.1	41
249	Solution Synthesis Approach to Colloidal Cesium Lead Halide Perovskite Nanoplatelets with Monolayer-Level Thickness Control. *Journal of the American Chemical Society*, **2016**, 138, 1010-6	16.4	615

248	Chapter 8:First Principles Modeling of Perovskite Solar Cells: Interplay of Structural, Electronic and Dynamical Effects. *RSC Energy and Environment Series*, **2016**, 234-296	0.6	2
247	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	13.4	141
246	Enhanced TiO2/MAPbI3 Electronic Coupling by Interface Modification with PbI2. *Chemistry of Materials*, **2016**, 28, 3612-3615	9.6	54
245	Mobile Ions in Organohalide Perovskites: Interplay of Electronic Structure and Dynamics. *ACS Energy Letters*, **2016**, 1, 182-188	20.1	143
244	Optical absorption spectrum of the N3 solar cell sensitizer by second-order multireference perturbation theory. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	10
243	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, 1638-45	6.4	220
242	High Open-Circuit Voltage: Fabrication of Formamidinium Lead Bromide Perovskite Solar Cells Using FluoreneDithiophene Derivatives as Hole-Transporting Materials. *ACS Energy Letters*, **2016**, 1, 107-112	20.1	92
241	Electronic and optical properties of MAPbX perovskites (X = I, Br, Cl): a unified DFT and GW theoretical analysis. *Physical Chemistry Chemical Physics*, **2016**, 18, 27158-27164	3.6	108
240	Vibrational Response of Methylammonium Lead Iodide: From Cation Dynamics to Phonon-Phonon Interactions. *ChemSusChem*, **2016**, 9, 2994-3004	8.3	38
239	Permanent excimer superstructures by supramolecular networking of metal quantum clusters. *Science*, **2016**, 353, 571-5	33.3	43
238	First-Principles Modeling of Organohalide Thin Films and Interfaces **2016**, 19-52		4
237	The effect of TiO2 surface on the electron injection efficiency in PbS quantum dot solar cells: a first-principles study. *Physical Chemistry Chemical Physics*, **2015**, 17, 6076-86	3.6	18
236	Structural and electronic properties of photoexcited TiO2 nanoparticles from first principles. *Journal of Chemical Theory and Computation*, **2015**, 11, 635-45	6.4	28
235	Structural and electronic properties of organo-halide hybrid perovskites from ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2015**, 17, 9394-409	3.6	116
234	Quantitative structureProperty relationship modeling of ruthenium sensitizers for solar cells applications: novel tools for designing promising candidates. *RSC Advances*, **2015**, 5, 23865-23873	3.7	13
233	Science in the Age of Digital Networking. *Journal of Physical Chemistry Letters*, **2015**, 6, 2900-1	6.4	
232	Monitoring the intramolecular charge transfer process in the Z907 solar cell sensitizer: a transient Vis and IR spectroscopy and ab initio investigation. *Physical Chemistry Chemical Physics*, **2015**, 17, 21594-604	3.6	10
231	Ab Initio Molecular Dynamics Simulations of Methylammonium Lead Iodide Perovskite Degradation by Water. *Chemistry of Materials*, **2015**, 27, 4885-4892	9.6	323

230	Thermal Fluctuations on Förster 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	3.8	6
229	Energy Level Alignment at Titanium Oxide/Dye Interfaces: Implications for Electron Injection and Light Harvesting. *Journal of Physical Chemistry C*, **2015**, 119, 9899-9909	3.8	25
228	Modeling Mesoporous Nanoparticulated TiO2 Films through Nanopolyhedra Random Packing. *Journal of Physical Chemistry C*, **2015**, 119, 10716-10726	3.8	3
227	First-Principles Modeling of a Dye-Sensitized TiO2/IrO2 Photoanode for Water Oxidation. *Journal of the American Chemical Society*, **2015**, 137, 5798-809	16.4	50
226	Carbazole-based sensitizers for potential application to dye sensitized solar cells. *Journal of Chemical Sciences*, **2015**, 127, 383-394	1.8	15
225	First-Principles Modeling of Core/Shell Quantum Dot Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2015**, 119, 12739-12748	3.8	19
224	Photoinduced Energy Shift in Quantum-Dot-Sensitized TiO2: A First-Principles Analysis. *Journal of Physical Chemistry Letters*, **2015**, 6, 1423-9	6.4	10
223	Intrinsic Thermal Instability of Methylammonium Lead Trihalide Perovskite. *Advanced Energy Materials*, **2015**, 5, 1500477	21.8	1386
222	Ligand Induced Spectral Changes in CdSe Quantum Dots. *ACS Applied Materials & Interfaces*, **2015**, 7, 19736-45	9.5	46
221	CHNHPbI perovskite single crystals: surface photophysics and their interaction with the environment. *Chemical Science*, **2015**, 6, 7305-7310	9.4	171
220	Water Oxidation by the [Co4O4(OAc)4(py)4](+) Cubium is Initiated by OH(-) Addition. *Journal of the American Chemical Society*, **2015**, 137, 15460-8	16.4	58
219	Effect of the anchoring group in the performance of carbazole-phenothiazine dyads for dye-sensitized solar cells. *Dyes and Pigments*, **2015**, 113, 536-545	4.6	27
218	Triphenylamine-functionalized corrole sensitizers for solar-cell applications. *Physica Status Solidi (A) Applications and Materials Science*, **2015**, 212, 194-202	1.6	25
217	New thiocyanate-free ruthenium(II) sensitizers with different pyrid-2-yl tetrazolate ligands for dye-sensitized solar cells. *Dalton Transactions*, **2015**, 44, 11788-96	4.3	24
216	Photoinduced Reversible Structural Transformations in Free-Standing CH3NH3PbI3 Perovskite Films. *Journal of Physical Chemistry Letters*, **2015**, 6, 2332-8	6.4	172
215	Origin of the Thermal Instability in CH3NH3PbI3 Thin Films Deposited on ZnO. *Chemistry of Materials*, **2015**, 27, 4229-4236	9.6	448
214	Ferroelectric Polarization of CH3NH3PbI3: A Detailed Study Based on Density Functional Theory and Symmetry Mode Analysis. *Journal of Physical Chemistry Letters*, **2015**, 6, 2223-31	6.4	151
213	Defect migration in methylammonium lead iodide and its role in perovskite solar cell operation. *Energy and Environmental Science*, **2015**, 8, 2118-2127	35.4	1003

212	Benzodithiophene based organic dyes for DSSC: Effect of alkyl chain substitution on dye efficiency. *Dyes and Pigments*, **2015**, 121, 351-362	4.6	19
211	Electronic and optical properties of mixed Sn□Pb organohalide perovskites: a first principles investigation. *Journal of Materials Chemistry A*, **2015**, 3, 9208-9215	13	156
210	Functionalized Ruthenium Dialkynyl Complexes with High Second-Order Nonlinear Optical Properties and Good Potential as Dye Sensitizers for Solar Cells. *Organometallics*, **2015**, 34, 94-104	3.8	25
209	Novel heteroleptic Ru(II) complexes: synthesis, characterization and application in dye-sensitized solar cells. *Dalton Transactions*, **2015**, 44, 5369-78	4.3	10
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