

Filippo De Angelis

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34,791
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ext. papers

38,449
ext. citations

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L-index

#	Paper	IF	Citations
373	Combined experimental and DFT-TDDFT computational study of photoelectrochemical cell ruthenium sensitizers. <i>Journal of the American Chemical Society</i> , 2005 , 127, 16835-47	16.4	2503
372	Intrinsic Thermal Instability of Methylammonium Lead Trihalide Perovskite. <i>Advanced Energy Materials</i> , 2015 , 5, 1500477	21.8	1386
371	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
370	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
369	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
368	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
367	Molecular engineering of organic sensitizers for solar cell applications. <i>Journal of the American Chemical Society</i> , 2006 , 128, 16701-7	16.4	728
366	A molecularly engineered hole-transporting material for efficient perovskite solar cells. <i>Nature Energy</i> , 2016 , 1,	62.3	693
365	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
364	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
363	Molecular engineering of organic sensitizers for dye-sensitized solar cell applications. <i>Journal of the American Chemical Society</i> , 2008 , 130, 6259-66	16.4	595
362	Titanium dioxide nanomaterials for photovoltaic applications. <i>Chemical Reviews</i> , 2014 , 114, 10095-130	68.1	567
361	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
360	Efficient far red sensitization of nanocrystalline TiO ₂ films by an unsymmetrical squaraine dye. <i>Journal of the American Chemical Society</i> , 2007 , 129, 10320-1	16.4	466
359	Stabilizing halide perovskite surfaces for solar cell operation with wide-bandgap lead oxysalts. <i>Science</i> , 2019 , 365, 473-478	33.3	460
358	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
357	Migration of cations induces reversible performance losses over day/night cycling in perovskite solar cells. <i>Energy and Environmental Science</i> , 2017 , 10, 604-613	35.4	387

356	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
355	Large polarons in lead halide perovskites. <i>Science Advances</i> , 2017 , 3, e1701217	14.3	374
354	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	35.4	355
353	Iodine chemistry determines the defect tolerance of lead-halide perovskites. <i>Energy and Environmental Science</i> , 2018 , 11, 702-713	35.4	353
352	Influence of the sensitizer adsorption mode on the open-circuit potential of dye-sensitized solar cells. <i>Nano Letters</i> , 2007 , 7, 3189-95	11.5	325
351	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
350	Theoretical studies on anatase and less common TiO ₂ phases: bulk, surfaces, and nanomaterials. <i>Chemical Reviews</i> , 2014 , 114, 9708-53	68.1	310
349	Defect-Assisted Photoinduced Halide Segregation in Mixed-Halide Perovskite Thin Films. <i>ACS Energy Letters</i> , 2017 , 2, 1416-1424	20.1	307
348	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
347	Absorption spectrum and solvatochromism of the [Ru(4,4'-COOH-2,2'-bpy) ₂ (NCS) ₂] molecular dye by time dependent density functional theory. <i>Journal of the American Chemical Society</i> , 2003 , 125, 4381-7	16.4	289
346	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
345	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
344	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
343	Light-induced annihilation of Frenkel defects in organo-lead halide perovskites. <i>Energy and Environmental Science</i> , 2016 , 9, 3180-3187	35.4	243
342	Alignment of the dye's molecular levels with the TiO ₂ band edges in dye-sensitized solar cells: a DFT-TDDFT study. <i>Nanotechnology</i> , 2008 , 19, 424002	3.4	230
341	Aggregation of organic dyes on TiO ₂ in dye-sensitized solar cells models: an ab initio investigation. <i>ACS Nano</i> , 2010 , 4, 556-62	16.7	229
340	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
339	Controlling phosphorescence color and quantum yields in cationic iridium complexes: a combined experimental and theoretical study. <i>Inorganic Chemistry</i> , 2007 , 46, 5989-6001	5.1	226

338	Fluorescent Alloy CsPb Mn I Perovskite Nanocrystals with High Structural and Optical Stability. <i>ACS Energy Letters</i> , 2017 , 2, 2183-2186	20.1	224
337	High open-circuit voltage solid-state dye-sensitized solar cells with organic dye. <i>Nano Letters</i> , 2009 , 9, 2487-92	11.5	220
336	Time-dependent density functional theory investigations on the excited states of Ru(II)-dye-sensitized TiO ₂ nanoparticles: the role of sensitizer protonation. <i>Journal of the American Chemical Society</i> , 2007 , 129, 14156-7	16.4	220
335	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
334	The Impact of the Crystallization Processes on the Structural and Optical Properties of Hybrid Perovskite Films for Photovoltaics. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3836-42	6.4	218
333	Influence of the dye molecular structure on the TiO ₂ conduction band in dye-sensitized solar cells: disentangling charge transfer and electrostatic effects. <i>Energy and Environmental Science</i> , 2013 , 6, 183-193	35.4	217
332	Synthesis, characterization, and DFT/TD-DFT calculations of highly phosphorescent blue light-emitting anionic iridium complexes. <i>Inorganic Chemistry</i> , 2008 , 47, 980-9	5.1	212
331	Time-dependent DFT study of [Fe(CN) ₆] ⁴⁻ sensitization of TiO ₂ nanoparticles. <i>Journal of the American Chemical Society</i> , 2004 , 126, 15024-5	16.4	210
330	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
329	Electronic transitions involved in the absorption spectrum and dual luminescence of tetranuclear cubane [Cu ₄ I ₄ (pyridine) ₄] cluster: a density functional theory/time-dependent density functional theory investigation. <i>Inorganic Chemistry</i> , 2006 , 45, 10576-84	5.1	200
328	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
327	First-Principles Modeling of the Adsorption Geometry and Electronic Structure of Ru(II) Dyes on Extended TiO ₂ Substrates for Dye-Sensitized Solar Cell Applications. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 6054-6061	3.8	192
326	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
325	Stark effect in perovskite/TiO ₂ solar cells: evidence of local interfacial order. <i>Nano Letters</i> , 2014 , 14, 2168-74	11.5	182
324	Di-branched di-anchoring organic dyes for dye-sensitized solar cells. <i>Energy and Environmental Science</i> , 2009 , 2, 1094	35.4	175
323	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
322	Ligand-engineered bandgap stability in mixed-halide perovskite LEDs. <i>Nature</i> , 2021 , 591, 72-77	50.4	172
321	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

320	Computational modelling of TiO ₂ surfaces sensitized by organic dyes with different anchoring groups: adsorption modes, electronic structure and implication for electron injection/recombination. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 920-8	3.6	165
319	Controlling competing photochemical reactions stabilizes perovskite solar cells. <i>Nature Photonics</i> , 2019 , 13, 532-539	33.9	161
318	Elusive Presence of Chloride in Mixed Halide Perovskite Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3532-8	6.4	160
317	The role of substituents on functionalized 1,10-phenanthroline in controlling the emission properties of cationic iridium(III) complexes of interest for electroluminescent devices. <i>Inorganic Chemistry</i> , 2007 , 46, 8533-47	5.1	160
316	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
315	First-Principles Modeling of Defects in Lead Halide Perovskites: Best Practices and Open Issues. <i>ACS Energy Letters</i> , 2018 , 3, 2206-2222	20.1	152
314	Ferroelectric Polarization of CH ₃ NH ₃ PbI ₃ : A Detailed Study Based on Density Functional Theory and Symmetry Mode Analysis. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 2223-31	6.4	151
313	Synthesis, characterization, and DFT-TDDFT computational study of a ruthenium complex containing a functionalized tetradentate ligand. <i>Inorganic Chemistry</i> , 2006 , 45, 4642-53	5.1	147
312	A computational approach to the electronic and optical properties of Ru(II) and Ir(III) polypyridyl complexes: Applications to DSC, OLED and NLO. <i>Coordination Chemistry Reviews</i> , 2011 , 255, 2704-2726	23.2	143
311	Mobile Ions in Organohalide Perovskites: Interplay of Electronic Structure and Dynamics. <i>ACS Energy Letters</i> , 2016 , 1, 182-188	20.1	143
310	Organic dyes incorporating low-band-gap chromophores based on extended benzothiadiazole for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2011 , 91, 192-198	4.6	142
309	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
308	Joint electrical, photophysical and computational studies on D-πA dye sensitized solar cells: the impacts of dithiophene rigidification. <i>Chemical Science</i> , 2012 , 3, 976	9.4	137
307	Energy levels, charge injection, charge recombination and dye regeneration dynamics for donor-acceptor conjugated organic dyes in mesoscopic TiO ₂ sensitized solar cells. <i>Energy and Environmental Science</i> , 2011 , 4, 1820	35.4	137
306	Calculation of near-edge x-ray-absorption fine structure at finite temperatures: spectral signatures of hydrogen bond breaking in liquid water. <i>Journal of Chemical Physics</i> , 2004 , 120, 8632-7	3.9	137
305	Formation of Surface Defects Dominates Ion Migration in Lead-Halide Perovskites. <i>ACS Energy Letters</i> , 2019 , 4, 779-785	20.1	135
304	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
303	Influence of Surface Termination on the Energy Level Alignment at the CH ₃ NH ₃ PbI ₃ Perovskite/C60 Interface. <i>Chemistry of Materials</i> , 2017 , 29, 958-968	9.6	119

302	Defect Activity in Lead Halide Perovskites. <i>Advanced Materials</i> , 2019 , 31, e1901183	24	119
301	Coumarin dyes containing low-band-gap chromophores for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2011 , 90, 304-310	4.6	119
300	Time-dependent density functional theory study of the absorption spectrum of [Ru(4,4'-COOH-2,2'-bpy) ₂ (NCS) ₂] in water solution: influence of the pH. <i>Chemical Physics Letters</i> , 2004 , 389, 204-208	2.5	118
299	Modeling Excited States and Alignment of Energy Levels in Dye-Sensitized Solar Cells: Successes, Failures, and Challenges. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 3685-3700	3.8	117
298	Ab Initio Determination of Ground and Excited State Oxidation Potentials of Organic Chromophores for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 22742-22750	3.8	117
297	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
296	Electronic and Optical Properties of the Spiro-MeOTAD Hole Conductor in Its Neutral and Oxidized Forms: A DFT/TDDFT Investigation. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 23126-23133	3.8	115
295	Direct vs. indirect injection mechanisms in perylene dye-sensitized solar cells: A DFT/TDDFT investigation. <i>Chemical Physics Letters</i> , 2010 , 493, 323-327	2.5	110
294	Photophysical properties of [Ru(phen) ₂ (dppz)] ²⁺ intercalated into DNA: an integrated Car-Parrinello and TDDFT study. <i>Journal of the American Chemical Society</i> , 2005 , 127, 14144-5	16.4	109
293	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
292	Modeling materials and processes in hybrid/organic photovoltaics: from dye-sensitized to perovskite solar cells. <i>Accounts of Chemical Research</i> , 2014 , 47, 3349-60	24.3	104
291	Electron-rich heteroaromatic conjugated bipyridine based ruthenium sensitizer for efficient dye-sensitized solar cells. <i>Chemical Communications</i> , 2008 , 5318-20	5.8	101
290	Solvent effects on the UV (n → π*) and NMR (13C and 17O) spectra of acetone in aqueous solution. An integrated car-parrinello and DFT/PCM approach. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 445-53	3.4	101
289	Electronic structure and reactivity of isomeric oxo-Mn(V) porphyrins: effects of spin-state crossing and pKa modulation. <i>Inorganic Chemistry</i> , 2006 , 45, 4268-76	5.1	101
288	Simulating Dye-Sensitized TiO ₂ Heterointerfaces in Explicit Solvent: Absorption Spectra, Energy Levels, and Dye Desorption. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 813-817	6.4	92
287	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
286	Ionotronic Halide Perovskite Drift-Diffusive Synapses for Low-Power Neuromorphic Computation. <i>Advanced Materials</i> , 2018 , 30, e1805454	24	91
285	Large electrostrictive response in lead halide perovskites. <i>Nature Materials</i> , 2018 , 17, 1020-1026	27	89

284	Cyclometalated iridium(III) complexes based on phenyl-imidazole ligand. <i>Inorganic Chemistry</i> , 2011 , 50, 451-62	5.1	87
283	Origin of low electron-hole recombination rate in metal halide perovskites. <i>Energy and Environmental Science</i> , 2018 , 11, 101-105	35.4	86
282	Mechanism of Reversible Trap Passivation by Molecular Oxygen in Lead-Halide Perovskites. <i>ACS Energy Letters</i> , 2017 , 2, 2794-2798	20.1	86
281	Time dependent density functional theory study of the absorption spectrum of the [Ru(4,4'-COOEt ₂ -bpy) ₂ (X) ₂] ⁴⁺ [X = NCS, Cl] dyes in water solution. <i>Chemical Physics Letters</i> , 2005 , 415, 115-120	2.5	86
280	Novel carbazole-phenothiazine dyads for dye-sensitized solar cells: a combined experimental and theoretical study. <i>ACS Applied Materials & Interfaces</i> , 2013 , 5, 9635-47	9.5	85
279	White-light phosphorescence emission from a single molecule: application to OLED. <i>Chemical Communications</i> , 2009 , 4672-4	5.8	85
278	Computational Investigation of Dye-Ligand Interactions in Organic Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 5965-5973	3.8	82
277	A TDDFT study of the ruthenium(II) polycyclic aromatic complex [Ru(dppz)(phen) ₂] ²⁺ in solution. <i>Chemical Physics Letters</i> , 2004 , 396, 43-48	2.5	81
276	Time-dependent density functional theory study of squaraine dye-sensitized solar cells. <i>Chemical Physics Letters</i> , 2009 , 475, 49-53	2.5	79
275	Cyclometalated iridium(III) complexes with substituted 1,10-phenanthrolines: a new class of highly active organometallic second order NLO-phores with excellent transparency with respect to second harmonic emission. <i>Chemical Communications</i> , 2007 , 4116-8	5.8	79
274	Terpyridine Zn(II), Ru(III), and Ir(III) complexes: the relevant role of the nature of the metal ion and of the ancillary ligands on the second-order nonlinear response of terpyridines carrying electron donor or electron acceptor groups. <i>Inorganic Chemistry</i> , 2005 , 44, 8967-78	5.1	79
273	A combined computational and experimental study of polynuclear Ru-TPPZ complexes: insight into the electronic and optical properties of coordination polymers. <i>Journal of the American Chemical Society</i> , 2004 , 126, 9715-23	16.4	78
272	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
271	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
270	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
269	Electrochemical Hole Injection Selectively Expels Iodide from Mixed Halide Perovskite Films. <i>Journal of the American Chemical Society</i> , 2019 , 141, 10812-10820	16.4	73
268	Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. <i>Chemical Physics</i> , 2009 , 358, 245-257	2.3	72
267	Intermolecular Interactions in Dye-Sensitized Solar Cells: A Computational Modeling Perspective. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 956-74	6.4	71

266	Absorption and emission of the apigenin and luteolin flavonoids: a TDDFT investigation. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 15118-26	2.8	70
265	Optical Properties and Aggregation of Phenothiazine-Based Dye-Sensitizers for Solar Cells Applications: A Combined Experimental and Computational Investigation. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 9613-9622	3.8	69
264	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
263	Interplay of stereoelectronic and environmental effects in tuning the structural and magnetic properties of a prototypical spin probe: further insights from a first principle dynamical approach. <i>Journal of the American Chemical Society</i> , 2006 , 128, 4338-47	16.4	68
262	Globularity-Selected Large Molecules for a New Generation of Multication Perovskites. <i>Advanced Materials</i> , 2017 , 29, 1702005	24	67
261	Instability of Tin Iodide Perovskites: Bulk p-Doping versus Surface Tin Oxidation. <i>ACS Energy Letters</i> , 2020 , 5, 2787-2795	20.1	67
260	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
259	Ligand Engineering for the Efficient Dye-Sensitized Solar Cells with Ruthenium Sensitizers and Cobalt Electrolytes. <i>Inorganic Chemistry</i> , 2016 , 55, 6653-9	5.1	65
258	Engineering of thiocyanate-free Ru(II) sensitizers for high efficiency dye-sensitized solar cells. <i>Chemical Science</i> , 2013 , 4, 2423	9.4	65
257	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
256	Tin versus Lead Redox Chemistry Modulates Charge Trapping and Self-Doping in Tin/Lead Iodide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 3546-3556	6.4	64
255	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
254	Cyclometalated Ir(III) complexes with substituted 1,10-phenanthrolines: a new class of efficient cationic organometallic second-order NLO chromophores. <i>Chemistry - A European Journal</i> , 2010 , 16, 4814-25	4.8	60
253	Influence of Donor Groups of Organic Dye on Open-Circuit Voltage in Solid-State Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 1572-1578	3.8	59
252	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
251	Ultrafast THz Probe of Photoinduced Polarons in Lead-Halide Perovskites. <i>Physical Review Letters</i> , 2019 , 122, 166601	7.4	56
250	Luminescent cyclometalated Ir(III) and Pt(II) complexes with beta-diketonate ligands as highly active second-order NLO chromophores. <i>Chemical Communications</i> , 2010 , 46, 2414-6	5.8	56
249	Tetraaryl Zn(II) porphyrinates substituted at meso-pyrrolic positions as sensitizers in dye-sensitized solar cells: a comparison with meso-disubstituted push-pull Zn(II) porphyrinates. <i>Chemistry - A European Journal</i> , 2013 , 19, 10723-40	4.8	55

248	Tuning the photoinduced O ₂ -evolving reactivity of Mn ⁴ O ₄ 7 ⁺ , Mn ⁴ O ₄ 6 ⁺ , and Mn ⁴ O ₃ (OH) ₆ ⁺ manganese-oxo cubane complexes. <i>Inorganic Chemistry</i> , 2006 , 45, 189-95	5.1	54
247	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
246	Computational Modeling of Stark Effects in Organic Dye-Sensitized TiO ₂ Heterointerfaces. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 1261-7	6.4	53
245	Modeling Ruthenium-Dye-Sensitized TiO ₂ Surfaces Exposing the (001) or (101) Faces: A First-Principles Investigation. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 18124-18131	3.8	52
244	Panchromatic ruthenium sensitizer based on electron-rich heteroarylvinylene π -conjugated quaterpyridine for dye-sensitized solar cells. <i>Dalton Transactions</i> , 2011 , 40, 234-42	4.3	52
243	Modeling ZnS and ZnO Nanostructures: Structural, Electronic, and Optical Properties. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 25219-25226	3.8	51
242	First-Principles Modeling of a Dye-Sensitized TiO ₂ /IrO ₂ Photoanode for Water Oxidation. <i>Journal of the American Chemical Society</i> , 2015 , 137, 5798-809	16.4	50
241	Stable Ligand Coordination at the Surface of Colloidal CsPbBr ₃ Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 3715-3726	6.4	49
240	From Large to Small Polarons in Lead, Tin, and Mixed Lead-Tin Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 1790-1798	6.4	49
239	Optical properties of ZnO nanostructures: a hybrid DFT/TDDFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 467-75	3.6	49
238	Panchromatic cross-substituted squaraines for dye-sensitized solar cell applications. <i>ChemSusChem</i> , 2009 , 2, 621-4	8.3	49
237	Quantum chemical evaluation of protein control over heme ligation: CO/O ₂ discrimination in myoglobin. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 3065-70	3.4	49
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