

# Alessandro Mattoni

## 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.

105  
papers

3,070  
citations

33  
h-index

52  
g-index

109  
ext. papers

3,486  
ext. citations

6.7  
avg, IF

5.53  
L-index

#	Paper	IF	Citations
105	Remarkably Weak Anisotropy in Thermal Conductivity of Two-Dimensional Hybrid Perovskite Butylammonium Lead Iodide Crystals. <i>Nano Letters</i> , <b>2021</b> , 21, 3708-3714	11.5	9
104	Theoretical insight on PTB7:PC71BM, PTB7-th:PC71BM and Si-PCPDTBT:PC71BM interactions governing blend nanoscale morphology for efficient solar cells. <i>Nano Energy</i> , <b>2021</b> , 82, 105708	17.1	3
103	Crystal-Size-Induced Band Gap Tuning in Perovskite Films. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 21368-21376	16.4	3
102	Crystal-Size-Induced Band Gap Tuning in Perovskite Films. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 21538-21546	3.6	3
101	Fundamentals of tin iodide perovskites: a promising route to highly efficient, lead-free solar cells. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 11812-11826	13	12
100	Long-lived electrets and lack of ferroelectricity in methylammonium lead bromide CH <sub>3</sub> NH <sub>2</sub> PbBr <sub>3</sub> ferroelastic single crystals. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 3233-3245	3.6	4
99	Direct Correlation of Nanoscale Morphology and Device Performance to Study Photocurrent Generation in Donor-Enriched Phases of Polymer Solar Cells. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 28404-28415	9.5	3
98	Ion Migration-Induced Amorphization and Phase Segregation as a Degradation Mechanism in Planar Perovskite Solar Cells. <i>Advanced Energy Materials</i> , <b>2020</b> , 10, 2000310	21.8	56
97	Dielectric function of hybrid perovskites at finite temperature investigated by classical molecular dynamics. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 104705	3.9	5
96	Ultralow Thermal Conductivity of Two-Dimensional Metal Halide Perovskites. <i>Nano Letters</i> , <b>2020</b> , 20, 3331-3337	11.5	38
95	Ag/In lead-free double perovskites. <i>EcoMat</i> , <b>2020</b> , 2, e12017	9.4	12
94	The dominant role of surfaces in the hysteretic behavior of hybrid perovskites. <i>Nano Energy</i> , <b>2020</b> , 67, 104162	17.1	12
93	Machine-Learned Charge Transfer Integrals for Multiscale Simulations in Organic Thin Films. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 17733-17743	3.8	12
92	Defect Dynamics in MAPbI <sub>3</sub> Polycrystalline Films: The Trapping Effect of Grain Boundaries. <i>Helvetica Chimica Acta</i> , <b>2020</b> , 103, e2000110	2	3
91	The Role of Grain Boundaries on Ionic Defect Migration in Metal Halide Perovskites. <i>Advanced Energy Materials</i> , <b>2020</b> , 10, 1903735	21.8	52
90	Layered Germanium Hybrid Perovskite Bromides: Insights from Experiments and First-Principles Calculations. <i>Advanced Functional Materials</i> , <b>2019</b> , 29, 1903528	15.6	17
89	Dual effect of humidity on cesium lead bromide: enhancement and degradation of perovskite films. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 12292-12302	13	46

88	Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Perovskites. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 6753-6762	3.8	2
87	Machine Learning-Based Charge Transport Computation for Pentacene. <i>Advanced Theory and Simulations</i> , <b>2019</b> , 2, 1800136	3.5	18
86	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. <i>Advanced Materials Interfaces</i> , <b>2018</b> , 6, 1801173	4.6	13
85	Development of a Classical Interatomic Potential for MAPbBr <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 3724-3733	3.8	19
84	Self-Assembled Lead Halide Perovskite Nanocrystals in a Perovskite Matrix. <i>ACS Energy Letters</i> , <b>2017</b> , 2, 769-775	20.1	12
83	Confinement of vibrational modes within crystalline lattices using thin amorphous layers. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 145302	1.8	
82	Collective Molecular Mechanisms in the CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Dissolution by Liquid Water. <i>ACS Nano</i> , <b>2017</b> , 11, 9183-9190	11.7	49
81	Linking morphology to thermal conductivity in PEDOT: an atomistic investigation. <i>Journal Physics D: Applied Physics</i> , <b>2017</b> , 50, 494002	3	13
80	Photoluminescence, optical gain, and lasing threshold in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> methylammonium lead-halide perovskites obtained by ab initio calculations. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 12758-12768	7.1	4
79	Toward High-Temperature Stability of PTB7-Based Bulk Heterojunction Solar Cells: Impact of Fullerene Size and Solvent Additive. <i>Advanced Energy Materials</i> , <b>2017</b> , 7, 1601486	21.8	46
78	Modeling hybrid perovskites by molecular dynamics. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 043008	0.8	45
77	Bulk Structural and Electronic Properties at the Density Functional Theory and Post-Density Functional Theory Level of Calculation <b>2017</b> , 43-86		
76	Structure and Thermodynamic Properties of Hybrid Perovskites by Classical Molecular Dynamics <b>2017</b> , 1-42		
75	Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface. <i>ACS Energy Letters</i> , <b>2016</b> , 1, 454-463	20.1	39
74	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. <i>Science Advances</i> , <b>2016</b> , 2, e1601156	14.3	238
73	Thermally Activated Point Defect Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultrahigh Mobility of Iodine. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 2356-61	6.4	93
72	Temperature Evolution of Methylammonium Trihalide Vibrations at the Atomic Scale. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 529-35	6.4	66
71	Appealing Perspectives of Hybrid Lead Iodide Perovskites as Thermoelectric Materials. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 28472-28479	3.8	49

70	Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskites. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 15352-62	3.6	68
69	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 24318-24	3.6	41
68	The study of polythiophene/water interfaces by sum-frequency generation spectroscopy and molecular dynamics simulations. <i>Journal of Materials Chemistry B</i> , <b>2015</b> , 3, 6429-6438	7.3	17
67	Atomistic Modeling of Morphology and Electronic Properties of Colloidal Ultrathin Bi <sub>2</sub> S <sub>3</sub> Nanowires. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 16913-16919	3.8	11
66	Methylammonium Rotational Dynamics in Lead Halide Perovskite by Classical Molecular Dynamics: The Role of Temperature. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 17421-17428	3.8	200
65	Intrinsic origin of two-dimensional electron gas at the (001) surface of SrTiO <sub>3</sub> . <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	24
64	Competing Forces in the Self-Assembly of Coupled ZnO Nanopyramids. <i>ACS Nano</i> , <b>2015</b> , 9, 3685-94	16.7	20
63	Pinpointing the Cause of Platinum Tipping on CdS Nanorods. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 22663-22668	3.8	2
62	Entropy-Suppressed Ferroelectricity in Hybrid Lead-Iodide Perovskites. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 4909-15	6.4	47
61	Methylammonium fragmentation in amines as source of localized trap levels and the healing role of Cl in hybrid lead-iodide perovskites. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	53
60	Colloidal Bi <sub>2</sub> S <sub>3</sub> Nanocrystals: Quantum Size Effects and Midgap States. <i>Advanced Functional Materials</i> , <b>2014</b> , 24, 3341-3350	15.6	58
59	Effect of Thermodynamics and Curvature on the Crystallinity of P3HT Thin Films on ZnO: Insights from Atomistic Simulations. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 4687-4694	3.8	10
58	Atomistic simulations of P(NDI2OD-T2) morphologies: from single chain to condensed phases. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 12556-65	3.4	16
57	Effects of TIPS-functionalization and perhalogenation on the electronic, optical, and transport properties of angular and compact dibenzochrycene. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 5170-7	2.8	33
56	Radiative Recombination and Photoconversion of Methylammonium Lead Iodide Perovskite by First Principles: Properties of an Inorganic Semiconductor within a Hybrid Body. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 24843-24853	3.8	69
55	Interfacial Engineering of P3HT/ZnO Hybrid Solar Cells Using Phthalocyanines: A Joint Theoretical and Experimental Investigation. <i>Advanced Energy Materials</i> , <b>2014</b> , 4, 1301694	21.8	38
54	Carrier Localization in Nanocrystalline Silicon. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 13417-13423	3.8	9
53	Atomistic simulations of thiol-terminated modifiers for hybrid photovoltaic interfaces. <i>Thin Solid Films</i> , <b>2014</b> , 560, 34-38	2.2	1

52	Thermally induced recrystallization of textured hydrogenated nanocrystalline silicon. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	17
51	Colloidal synthesis and characterization of Bi <sub>2</sub> S <sub>3</sub> nanoparticles for photovoltaic applications. <i>Journal of Physics: Conference Series</i> , <b>2014</b> , 566, 012017	0.3	6
50	Hybrid perovskites for photovoltaics: Insights from first principles. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	168
49	Electronic Properties and Quantum Confinement in Bi <sub>2</sub> S <sub>3</sub> Ribbon-Like Nanostructures. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 21923-21929	3.8	14
48	Atomistic Investigation of the Solubility of 3-Alkylthiophene Polymers in Tetrahydrofuran Solvent. <i>Macromolecules</i> , <b>2013</b> , 46, 8003-8008	5.5	26
47	A (time-dependent) density functional theory study of the optoelectronic properties of bis-triisopropylsilylethynyl-functionalized acenes. <i>Thin Solid Films</i> , <b>2013</b> , 543, 32-34	2.2	6
46	Role of Molecular Thermodynamical Processes at Functionalized Polymer/Metaloxide Interfaces for Photovoltaics. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 13894-13901	3.8	11
45	Atomistic Investigation of the Solid-Liquid Interface between the Crystalline Zinc Oxide Surface and the Liquid Tetrahydrofuran Solvent. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 12644-12648	3.8	7
44	Structural and Optoelectronic Properties of Unsaturated ZnO and ZnS Nanoclusters. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 8741-8746	3.8	40
43	Optoelectronic properties of (ZnO) <sub>60</sub> isomers. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 14293-8	3.6	13
42	The effect of selective interactions at the interface of polymer-oxide hybrid solar cells. <i>Energy and Environmental Science</i> , <b>2012</b> , 5, 9068	35.4	42
41	Electronic Properties of Hybrid Zinc Oxide-Oligothiophene Nanostructures. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 8174-8180	3.8	13
40	Zinc Oxide-Zinc Phthalocyanine Interface for Hybrid Solar Cells. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 15439-15448	3.8	34
39	Self-assembling of zinc phthalocyanines on ZnO (1010) surface through multiple time scales. <i>ACS Nano</i> , <b>2011</b> , 5, 9639-47	16.7	12
38	Electronic and optical properties of families of polycyclic aromatic hydrocarbons: A systematic (time-dependent) density functional theory study. <i>Chemical Physics</i> , <b>2011</b> , 384, 19-27	2.3	114
37	Poly(3-hexylthiophene) Adhesion on Zinc Oxide Nanoneedles. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 16833-16837	3.8	18
36	Adhesion and Diffusion of Zinc-Phthalocyanines on the ZnO (101 0) Surface. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 18208-18212	3.8	8
35	Self-Assembling of Poly(3-hexylthiophene). <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 576-581	3.8	60

34	Polymer Crystallinity and Transport Properties at the Poly(3-hexylthiophene)/Zinc Oxide Interface. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 9651-9655	3.8	30
33	Brittle Fracture: From Elasticity Theory to Atomistic Simulations. <i>Reviews in Computational Chemistry</i> , <b>2010</b> , 1-83		3
32	Understanding the Helical Wrapping of Poly(3-hexylthiophene) on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 21109-21113	3.8	52
31	Atomistic Investigation of Poly(3-hexylthiophene) Adhesion on Nanostructured Titania. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 3401-3406	3.8	31
30	Quantum confinement by an order-disorder boundary in nanocrystalline silicon. <i>Physical Review Letters</i> , <b>2010</b> , 104, 176803	7.4	27
29	Calculation of the local optoelectronic properties of nanostructured silicon. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	3
28	Electronic localization and optical absorption in embedded silicon nanograins. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 053115	3.4	14
27	Crystallization kinetics of mixed amorphous-crystalline nanosystems. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	17
26	Atomistic fracture: QFM vs. MD. <i>Engineering Fracture Mechanics</i> , <b>2008</b> , 75, 1794-1803	4.2	17
25	Atomistic modeling of brittleness in covalent materials. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	30
24	Nonuniform growth of embedded silicon nanocrystals in an amorphous matrix. <i>Physical Review Letters</i> , <b>2007</b> , 99, 205501	7.4	18
23	Failure strength of brittle materials containing nanovoids. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	10
22	Role of lattice discreteness on brittle fracture: Atomistic simulations versus analytical models. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	42
21	Lattice strain induced by boron clusters in crystalline silicon. <i>Semiconductor Science and Technology</i> , <b>2006</b> , 21, L41-L44	1.8	15
20	Nanocrystalline silicon films as multifunctional material for optoelectronic and photovoltaic applications. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , <b>2006</b> , 134, 118-124	3.1	29
19	Atomic-Scale Investigation on Fracture Toughness in Nanocomposite Silicon Carbide <b>2006</b> , 41-42		
18	Analytical Approaches VS Atomistic Simulations in Fracture <b>2006</b> , 1105-1106		
17	Fracture toughness of nanostructured silicon carbide. <i>Applied Physics Letters</i> , <b>2005</b> , 87, 141912	3.4	14

16	Crack-tip stress shielding by a hard fiber in $\beta$ -SiC: an atomistic study. <i>Computer Physics Communications</i> , <b>2005</b> , 169, 40-43	4.2	
15	Computational Materials Science application programming interface (CMSapi): a tool for developing applications for atomistic simulations. <i>Computer Physics Communications</i> , <b>2005</b> , 169, 462-466 <sup>4.2</sup>	4.2	8
14	Atomic scale origin of crack resistance in brittle fracture. <i>Physical Review Letters</i> , <b>2005</b> , 95, 115501	7.4	71
13	Atomistic study of the dissolution of small boron interstitial clusters in c-Si. <i>Applied Physics Letters</i> , <b>2005</b> , 87, 191912	3.4	22
12	Energetics of native point defects in cubic silicon carbide. <i>European Physical Journal B</i> , <b>2004</b> , 38, 437-444 <sup>1.2</sup>	1.2	20
11	Defect energetics of $\beta$ -SiC using a new tight-binding molecular dynamics model. <i>Journal of Nuclear Materials</i> , <b>2004</b> , 329-333, 1219-1222	3.3	18
10	Boron ripening during solid-phase epitaxy of amorphous silicon. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	63
9	Atomistic study of the interaction between a microcrack and a hard inclusion in $\beta$ -SiC. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	22
8	Boron ripening in amorphous silicon by large scale molecular dynamics simulations. <i>Computational Materials Science</i> , <b>2004</b> , 30, 143-149	3.2	1
7	On the solid-phase epitaxy of the a-Si:B/c-Si interface. <i>Europhysics Letters</i> , <b>2003</b> , 62, 862-868	1.6	6
6	Ferromagnetic transitions of a spin-one Ising film in a surface and bulk transverse fields. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2002</b> , 251, 129-137	2.8	9
5	Interaction between self-interstitials and substitutional C in silicon: Interstitial trapping and C clustering mechanism. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	80
4	Self-interstitial trapping by carbon complexes in crystalline silicon. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	42
3	Modeling of Self-Interstitial Diffusion in Implanted Molecular Beam Epitaxy Silicon. <i>Materials Research Society Symposia Proceedings</i> , <b>2002</b> , 717, 1		5
2	Mean-field theory for Josephson junction arrays with charge frustration. <i>Physical Review B</i> , <b>2000</b> , 61, 11676-11688	3.3	17
1	Highly Emissive Layers based on Organic/Inorganic Nanohybrids Using Aggregation Induced Emission Effect. <i>Advanced Materials Technologies</i> , 2100876	6.8	2