Alessandro Mattoni

List of Publications by Citations

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	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. *Science Advances*, **2016**, 2, e1601156	14.3	238
104	Methylammonium Rotational Dynamics in Lead Halide Perovskite by Classical Molecular Dynamics: The Role of Temperature. *Journal of Physical Chemistry C*, **2015**, 119, 17421-17428	3.8	200
103	Hybrid perovskites for photovoltaics: Insights from first principles. *Physical Review B*, **2014**, 89,	3.3	168
102	Electronic and optical properties of families of polycyclic aromatic hydrocarbons: A systematic (time-dependent) density functional theory study. *Chemical Physics*, **2011**, 384, 19-27	2.3	114
101	Thermally Activated Point Defect Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultrahigh Mobility of Iodine. *Journal of Physical Chemistry Letters*, **2016**, 7, 2356-61	6.4	93
100	Interaction between self-interstitials and substitutional C in silicon: Interstitial trapping and C clustering mechanism. *Physical Review B*, **2002**, 65,	3.3	80
99	Atomic scale origin of crack resistance in brittle fracture. *Physical Review Letters*, **2005**, 95, 115501	7.4	71
98	Radiative Recombination and Photoconversion of Methylammonium Lead Iodide Perovskite by First Principles: Properties of an Inorganic Semiconductor within a Hybrid Body. *Journal of Physical Chemistry C*, **2014**, 118, 24843-24853	3.8	69
97	Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide CH3NH3PbI3 perovskites. *Physical Chemistry Chemical Physics*, **2016**, 18, 15352-62	3.6	68
96	Temperature Evolution of Methylammonium Trihalide Vibrations at the Atomic Scale. *Journal of Physical Chemistry Letters*, **2016**, 7, 529-35	6.4	66
95	Boron ripening during solid-phase epitaxy of amorphous silicon. *Physical Review B*, **2004**, 69,	3.3	63
94	Self-Assembling of Poly(3-hexylthiophene). *Journal of Physical Chemistry C*, **2011**, 115, 576-581	3.8	60
93	Colloidal Bi2S3 Nanocrystals: Quantum Size Effects and Midgap States. *Advanced Functional Materials*, **2014**, 24, 3341-3350	15.6	58
92	Ion Migration-Induced Amorphization and Phase Segregation as a Degradation Mechanism in Planar Perovskite Solar Cells. *Advanced Energy Materials*, **2020**, 10, 2000310	21.8	56
91	Methylammonium fragmentation in amines as source of localized trap levels and the healing role of Cl in hybrid lead-iodide perovskites. *Physical Review B*, **2015**, 92,	3.3	53
90	Understanding the Helical Wrapping of Poly(3-hexylthiophene) on Carbon Nanotubes. *Journal of Physical Chemistry C*, **2010**, 114, 21109-21113	3.8	52
89	The Role of Grain Boundaries on Ionic Defect Migration in Metal Halide Perovskites. *Advanced Energy Materials*, **2020**, 10, 1903735	21.8	52

88	Collective Molecular Mechanisms in the CHNHPbI Dissolution by Liquid Water. *ACS Nano*, **2017**, 11, 9183-9190	13.7	49
87	Appealing Perspectives of Hybrid Lead Iodide Perovskites as Thermoelectric Materials. *Journal of Physical Chemistry C*, **2016**, 120, 28472-28479	3.8	49
86	Entropy-Suppressed Ferroelectricity in Hybrid Lead-Iodide Perovskites. *Journal of Physical Chemistry Letters*, **2015**, 6, 4909-15	6.4	47
85	Dual effect of humidity on cesium lead bromide: enhancement and degradation of perovskite films. *Journal of Materials Chemistry A*, **2019**, 7, 12292-12302	13	46
84	Toward High-Temperature Stability of PTB7-Based Bulk Heterojunction Solar Cells: Impact of Fullerene Size and Solvent Additive. *Advanced Energy Materials*, **2017**, 7, 1601486	21.8	46
83	Modeling hybrid perovskites by molecular dynamics. *Journal of Physics Condensed Matter*, **2017**, 29, 043001	2.8	45
82	The effect of selective interactions at the interface of polymer oxide hybrid solar cells. *Energy and Environmental Science*, **2012**, 5, 9068	35.4	42
81	Role of lattice discreteness on brittle fracture: Atomistic simulations versus analytical models. *Physical Review B*, **2006**, 73,	3.3	42
80	Self-interstitial trapping by carbon complexes in crystalline silicon. *Physical Review B*, **2002**, 66,	3.3	42
79	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. *Physical Chemistry Chemical Physics*, **2016**, 18, 24318-24	3.6	41
78	Structural and Optoelectronic Properties of Unsaturated ZnO and ZnS Nanoclusters. *Journal of Physical Chemistry C*, **2012**, 116, 8741-8746	3.8	40
77	Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface. *ACS Energy Letters*, **2016**, 1, 454-463	20.1	39
76	Ultralow Thermal Conductivity of Two-Dimensional Metal Halide Perovskites. *Nano Letters*, **2020**, 20, 3331-3337	11.5	38
75	Interfacial Engineering of P3HT/ZnO Hybrid Solar Cells Using Phthalocyanines: A Joint Theoretical and Experimental Investigation. *Advanced Energy Materials*, **2014**, 4, 1301694	21.8	38
74	Zinc Oxide Zinc Phthalocyanine Interface for Hybrid Solar Cells. *Journal of Physical Chemistry C*, **2012**, 116, 15439-15448	3.8	34
73	Effects of TIPS-functionalization and perhalogenation on the electronic, optical, and transport properties of angular and compact dibenzochrysene. *Journal of Physical Chemistry A*, **2014**, 118, 5170-7	2.8	33
72	Atomistic Investigation of Poly(3-hexylthiophene) Adhesion on Nanostructured Titania. *Journal of Physical Chemistry C*, **2010**, 114, 3401-3406	3.8	31
71	Polymer Crystallinity and Transport Properties at the Poly(3-hexylthiophene)/Zinc Oxide Interface. *Journal of Physical Chemistry C*, **2011**, 115, 9651-9655	3.8	30

70	Atomistic modeling of brittleness in covalent materials. *Physical Review B*, **2007**, 76,	3.3	30
69	Nanocrystalline silicon films as multifunctional material for optoelectronic and photovoltaic applications. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2006**, 134, 118-124	3.1	29
68	Quantum confinement by an order-disorder boundary in nanocrystalline silicon. *Physical Review Letters*, **2010**, 104, 176803	7.4	27
67	Atomistic Investigation of the Solubility of 3-Alkylthiophene Polymers in Tetrahydrofuran Solvent. *Macromolecules*, **2013**, 46, 8003-8008	5.5	26
66	Intrinsic origin of two-dimensional electron gas at the (001) surface of SrTiO3. *Physical Review B*, **2015**, 91,	3.3	24
65	Atomistic study of the interaction between a microcrack and a hard inclusion in β-SiC. *Physical Review B*, **2004**, 70,	3.3	22
64	Atomistic study of the dissolution of small boron interstitial clusters in c-Si. *Applied Physics Letters*, **2005**, 87, 191912	3.4	22
63	Competing Forces in the Self-Assembly of Coupled ZnO Nanopyramids. *ACS Nano*, **2015**, 9, 3685-94	16.7	20
62	Energetics of native point defects in cubic silicon carbide. *European Physical Journal B*, **2004**, 38, 437-444	1.2	20
61	Development of a Classical Interatomic Potential for MAPbBr3. *Journal of Physical Chemistry C*, **2017**, 121, 3724-3733	3.8	19
60	Poly(3-hexylthiophene) Adhesion on Zinc Oxide Nanoneedles. *Journal of Physical Chemistry C*, **2011**, 115, 16833-16837	3.8	18
59	Nonuniform growth of embedded silicon nanocrystals in an amorphous matrix. *Physical Review Letters*, **2007**, 99, 205501	7.4	18
58	Defect energetics of β-SiC using a new tight-binding molecular dynamics model. *Journal of Nuclear Materials*, **2004**, 329-333, 1219-1222	3.3	18
57	Machine Learning–Based Charge Transport Computation for Pentacene. *Advanced Theory and Simulations*, **2019**, 2, 1800136	3.5	18
56	Layered Germanium Hybrid Perovskite Bromides: Insights from Experiments and First-Principles Calculations. *Advanced Functional Materials*, **2019**, 29, 1903528	15.6	17
55	The study of polythiophene/water interfaces by sum-frequency generation spectroscopy and molecular dynamics simulations. *Journal of Materials Chemistry B*, **2015**, 3, 6429-6438	7.3	17
54	Thermally induced recrystallization of textured hydrogenated nanocrystalline silicon. *Physical Review B*, **2014**, 89,	3.3	17
53	Crystallization kinetics of mixed amorphous-crystalline nanosystems. *Physical Review B*, **2008**, 78,	3.3	17

52	Atomistic fracture: QFM vs. MD. *Engineering Fracture Mechanics*, **2008**, 75, 1794-1803	4.2	17
51	Mean-field theory for Josephson junction arrays with charge frustration. *Physical Review B*, **2000**, 61, 11676-11688	3.3	17
50	Atomistic simulations of P(NDI2OD-T2) morphologies: from single chain to condensed phases. *Journal of Physical Chemistry B*, **2014**, 118, 12556-65	3.4	16
49	Lattice strain induced by boron clusters in crystalline silicon. *Semiconductor Science and Technology*, **2006**, 21, L41-L44	1.8	15
48	Electronic Properties and Quantum Confinement in Bi2S3 Ribbon-Like Nanostructures. *Journal of Physical Chemistry C*, **2013**, 117, 21923-21929	3.8	14
47	Electronic localization and optical absorption in embedded silicon nanograins. *Applied Physics Letters*, **2009**, 94, 053115	3.4	14
46	Fracture toughness of nanostructured silicon carbide. *Applied Physics Letters*, **2005**, 87, 141912	3.4	14
45	Linking morphology to thermal conductivity in PEDOT: an atomistic investigation. *Journal Physics D: Applied Physics*, **2017**, 50, 494002	3	13
44	Optoelectronic properties of (ZnO)60 isomers. *Physical Chemistry Chemical Physics*, **2012**, 14, 14293-8	3.6	13
43	Electronic Properties of Hybrid Zinc Oxide/Oligothiophene Nanostructures. *Journal of Physical Chemistry C*, **2012**, 116, 8174-8180	3.8	13
42	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. *Advanced Materials Interfaces*, **2018**, 6, 1801173	4.6	13
41	Self-Assembled Lead Halide Perovskite Nanocrystals in a Perovskite Matrix. *ACS Energy Letters*, **2017**, 2, 769-775	20.1	12
40	Ag/In lead-free double perovskites. *EcoMat*, **2020**, 2, e12017	9.4	12
39	Self-assembling of zinc phthalocyanines on ZnO (1010) surface through multiple time scales. *ACS Nano*, **2011**, 5, 9639-47	16.7	12
38	The dominant role of surfaces in the hysteretic behavior of hybrid perovskites. *Nano Energy*, **2020**, 67, 104162	17.1	12
37	Machine-Learned Charge Transfer Integrals for Multiscale Simulations in Organic Thin Films. *Journal of Physical Chemistry C*, **2020**, 124, 17733-17743	3.8	12
36	Fundamentals of tin iodide perovskites: a promising route to highly efficient, lead-free solar cells. *Journal of Materials Chemistry A*, **2021**, 9, 11812-11826	13	12
35	Atomistic Modeling of Morphology and Electronic Properties of Colloidal Ultrathin Bi2S3 Nanowires. *Journal of Physical Chemistry C*, **2015**, 119, 16913-16919	3.8	11

34	Role of Molecular Thermodynamical Processes at Functionalized Polymer/Metaloxide Interfaces for Photovoltaics. *Journal of Physical Chemistry C*, **2013**, 117, 13894-13901	3.8	11
33	Effect of Thermodynamics and Curvature on the Crystallinity of P3HT Thin Films on ZnO: Insights from Atomistic Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 4687-4694	3.8	10
32	Failure strength of brittle materials containing nanovoids. *Physical Review B*, **2007**, 75,	3.3	10
31	Carrier Localization in Nanocrystalline Silicon. *Journal of Physical Chemistry C*, **2014**, 118, 13417-13423	3.8	9
30	Ferromagnetic transitions of a spin-one Ising film in a surface and bulk transverse fields. *Journal of Magnetism and Magnetic Materials*, **2002**, 251, 129-137	2.8	9
29	Remarkably Weak Anisotropy in Thermal Conductivity of Two-Dimensional Hybrid Perovskite Butylammonium Lead Iodide Crystals. *Nano Letters*, **2021**, 21, 3708-3714	11.5	9
28	Adhesion and Diffusion of Zinc-Phthalocyanines on the ZnO (101 0) Surface. *Journal of Physical Chemistry C*, **2011**, 115, 18208-18212	3.8	8
27	Computational Materials Science application programming interface (CMSapi): a tool for developing applications for atomistic simulations. *Computer Physics Communications*, **2005**, 169, 462-466	4.2	8
26	Atomistic Investigation of the Solid□iquid Interface between the Crystalline Zinc Oxide Surface and the Liquid Tetrahydrofuran Solvent. *Journal of Physical Chemistry C*, **2012**, 116, 12644-12648	3.8	7
25	A (time-dependent) density functional theory study of the optoelectronic properties of bis-triisopropylsilylethynyl-functionalized acenes. *Thin Solid Films*, **2013**, 543, 32-34	2.2	6
24	Colloidal synthesis and characterization of Bi2S3nanoparticles for photovoltaic applications. *Journal of Physics: Conference Series*, **2014**, 566, 012017	0.3	6
23	On the solid-phase epitaxy of the a-Si:B/c-Si interface. *Europhysics Letters*, **2003**, 62, 862-868	1.6	6
22	Dielectric function of hybrid perovskites at finite temperature investigated by classical molecular dynamics. *Journal of Chemical Physics*, **2020**, 152, 104705	3.9	5
21	Modeling of Self-Interstitial Diffusion in Implanted Molecular Beam Epitaxy Silicon. *Materials Research Society Symposia Proceedings*, **2002**, 717, 1		5
20	Photoluminescence, optical gain, and lasing threshold in CH3NH3PbI3 methylammonium lead-halide perovskites obtained by ab initio calculations. *Journal of Materials Chemistry C*, **2017**, 5, 12758-12768	7.1	4
19	Long-lived electrets and lack of ferroelectricity in methylammonium lead bromide CHNHPbBr ferroelastic single crystals. *Physical Chemistry Chemical Physics*, **2021**, 23, 3233-3245	3.6	4
18	Direct Correlation of Nanoscale Morphology and Device Performance to Study Photocurrent Generation in Donor-Enriched Phases of Polymer Solar Cells. *ACS Applied Materials & Interfaces* , **2020**, 12, 28404-28415	9.5	3
17	Brittle Fracture: From Elasticity Theory to Atomistic Simulations. *Reviews in Computational Chemistry*, **2010**, 1-83		3

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16	Calculation of the local optoelectronic properties of nanostructured silicon. *Physical Review B*, **2009**, 79,	3.3	3
15	Defect Dynamics in MAPbI3 Polycrystalline Films: The Trapping Effect of Grain Boundaries. *Helvetica Chimica Acta*, **2020**, 103, e2000110	2	3
14	Theoretical insight on PTB7:PC71BM, PTB7-th:PC71BM and Si-PCPDTBT:PC71BM interactions governing blend nanoscale morphology for efficient solar cells. *Nano Energy*, **2021**, 82, 105708	17.1	3
13	Crystal-Size-Induced Band Gap Tuning in Perovskite Films. *Angewandte Chemie - International Edition*, **2021**, 60, 21368-21376	16.4	3
12	Crystal-Size-Induced Band Gap Tuning in Perovskite Films. *Angewandte Chemie*, **2021**, 133, 21538-21546	3.6	3
11	Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH3NH3PbI3 Perovskites. *Journal of Physical Chemistry C*, **2019**, 123, 6753-6762	3.8	2
10	Pinpointing the Cause of Platinum Tipping on CdS Nanorods. *Journal of Physical Chemistry C*, **2015**, 119, 22663-22668	3.8	2
9	Highly Emissive Layers based on Organic/Inorganic Nanohybrids Using Aggregation Induced Emission Effect. *Advanced Materials Technologies*,2100876	6.8	2
8	Atomistic simulations of thiol-terminated modifiers for hybrid photovoltaic interfaces. *Thin Solid Films*, **2014**, 560, 34-38	2.2	1
7	Boron ripening in amorphous silicon by large scale molecular dynamics simulations. *Computational Materials Science*, **2004**, 30, 143-149	3.2	1
6	Confinement of vibrational modes within crystalline lattices using thin amorphous layers. *Journal of Physics Condensed Matter*, **2017**, 29, 145302	1.8	
5	Crack-tip stress shielding by a hard fiber in SiC: an atomistic study. *Computer Physics Communications*, **2005**, 169, 40-43	4.2	
4	Atomic-Scale Investigation on Fracture Toughness in Nanocomposite Silicon Carbide **2006**, 41-42		
3	Anaytical Approaches VS Atomistic Simulations in Fracture **2006**, 1105-1106		
2	Bulk Structural and Electronic Properties at the Density Functional Theory and Post-Density Functional Theory Level of Calculation **2017**, 43-86		
1	Structure and Thermodynamic Properties of Hybrid Perovskites by Classical Molecular Dynamics **2017**, 1-42		