Alessandro Mattoni

List of Publications by Year
in descending order

106 papers	3,967 citations	117453 34 h-index	133063 59 g-index
109 all docs	109 docs citations	109 times ranked	5658 citing authors

#	Article	IF	Citations
1	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. Science Advances, 2016, 2, e1601156.	4.7	307
2	Methylammonium Rotational Dynamics in Lead Halide Perovskite by Classical Molecular Dynamics: The Role of Temperature. Journal of Physical Chemistry C, 2015, 119, 17421-17428.	1.5	255
3	Hybrid perovskites for photovoltaics: Insights from first principles. Physical Review B, 2014, 89, .	1.1	191
4	Electronic and optical properties of families of polycyclic aromatic hydrocarbons: A systematic (time-dependent) density functional theory study. Chemical Physics, 2011, 384, 19-27.	0.9	139
5	Thermally Activated Point Defect Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultrahigh Mobility of Iodine. Journal of Physical Chemistry Letters, 2016, 7, 2356-2361.	2.1	125
6	The Role of Grain Boundaries on Ionic Defect Migration in Metal Halide Perovskites. Advanced Energy Materials, 2020, 10, 1903735.	10.2	117
7	Ion Migrationâ€Induced Amorphization and Phase Segregation as a Degradation Mechanism in Planar Perovskite Solar Cells. Advanced Energy Materials, 2020, 10, 2000310.	10.2	103
8	Interaction between self-interstitials and substitutional C in silicon:â€ƒInterstitial trapping and C clustering mechanism. Physical Review B, 2002, 65, .	1.1	89
9	Atomic Scale Origin of Crack Resistance in Brittle Fracture. Physical Review Letters, 2005, 95, 115501.	2.9	83
10	Temperature Evolution of Methylammonium Trihalide Vibrations at the Atomic Scale. Journal of Physical Chemistry Letters, 2016, 7, 529-535.	2.1	82
11	Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide CH₃NH₃PbI₃perovskites. Physical Chemistry Chemical Physics, 2016, 18, 15352-15362.	1.3	77
12	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.	1.5	74
13	Dual effect of humidity on cesium lead bromide: enhancement and degradation of perovskite films. Journal of Materials Chemistry A, 2019, 7, 12292-12302.	5.2	74
14	Collective Molecular Mechanisms in the CH₃NH₃PbI₃ Dissolution by Liquid Water. ACS Nano, 2017, 11, 9183-9190.	7.3	73
15	Boron ripening during solid-phase epitaxy of amorphous silicon. Physical Review B, 2004, 69, .	1.1	67
16	Appealing Perspectives of Hybrid Leadâ€“Iodide Perovskites as Thermoelectric Materials. Journal of Physical Chemistry C, 2016, 120, 28472-28479.	1.5	66
17	Modeling hybrid perovskites by molecular dynamics. Journal of Physics Condensed Matter, 2017, 29, 043001.	0.7	66
18	Colloidal Bi₂S₃ Nanocrystals: Quantum Size Effects and Midgap States. Advanced Functional Materials, 2014, 24, 3341-3350.	7.8	65

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19	Self-Assembling of Poly(3-hexylthiophene). Journal of Physical Chemistry C, 2011, 115, 576-581.	1.5	64
20	Ultralow Thermal Conductivity of Two-Dimensional Metal Halide Perovskites. Nano Letters, 2020, 20, 3331-3337.	4.5	64
21	Understanding the Helical Wrapping of Poly(3-hexylthiophene) on Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 21109-21113.	1.5	55
22	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, .	1.1	54
23	Toward Highâ€Temperature Stability of PTB7â€Based Bulk Heterojunction Solar Cells: Impact of Fullerene Size and Solvent Additive. Advanced Energy Materials, 2017, 7, 1601486.	10.2	53
24	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. Physical Chemistry Chemical Physics, 2016, 18, 24318-24324.	1.3	52
25	Entropy-Suppressed Ferroelectricity in Hybrid Lead-Iodide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 4909-4915.	2.1	51
26	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, 5170-5177.	1.1	46
27	Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface. ACS Energy Letters, 2016, 1, 454-463.	8.8	46
28	Self-interstitial trapping by carbon complexes in crystalline silicon. Physical Review B, 2002, 66, .	1.1	45
29	Role of lattice discreteness on brittle fracture: Atomistic simulations versus analytical models. Physical Review B, 2006, 73, .	1.1	45
30	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. Advanced Materials Interfaces, 2019, 6, 1801173.	1.9	43
31	The effect of selective interactions at the interface of polymerâ€“oxide hybrid solar cells. Energy and Environmental Science, 2012, 5, 9068.	15.6	42
32	Interfacial Engineering of P3HT/ZnO Hybrid Solar Cells Using Phthalocyanines: A Joint Theoretical and Experimental Investigation. Advanced Energy Materials, 2014, 4, 1301694.	10.2	42
33	Structural and Optoelectronic Properties of Unsaturated ZnO and ZnS Nanoclusters. Journal of Physical Chemistry C, 2012, 116, 8741-8746.	1.5	41
34	Zinc Oxideâ€“Zinc Phthalocyanine Interface for Hybrid Solar Cells. Journal of Physical Chemistry C, 2012, 116, 15439-15448.	1.5	36
35	Atomistic modeling of brittleness in covalent materials. Physical Review B, 2007, 76, .	1.1	35
36	Rationalizing the design and implementation of chiral hybrid perovskites. CheM, 2022, 8, 1231-1253.	5.8	35

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37	Machine Learningâ€“Based Charge Transport Computation for Pentacene. Advanced Theory and Simulations, 2019, 2, 1800136.	1.3	34
38	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.	1.7	32
39	Atomistic Investigation of Poly(3-hexylthiophene) Adhesion on Nanostructured Titania. Journal of Physical Chemistry C, 2010, 114, 3401-3406.	1.5	32
40	Atomistic Investigation of the Solubility of 3-Alkylthiophene Polymers in Tetrahydrofuran Solvent. Macromolecules, 2013, 46, 8003-8008.	2.2	32
41	Fundamentals of tin iodide perovskites: a promising route to highly efficient, lead-free solar cells. Journal of Materials Chemistry A, 2021, 9, 11812-11826.	5.2	32
42	Development of a Classical Interatomic Potential for MAPbBr₃. Journal of Physical Chemistry C, 2017, 121, 3724-3733.	1.5	31
43	Quantum Confinement by an Order-Disorder Boundary in Nanocrystalline Silicon. Physical Review Letters, 2010, 104, 176803.	2.9	30
44	Polymer Crystallinity and Transport Properties at the Poly(3-hexylthiophene)/Zinc Oxide Interface. Journal of Physical Chemistry C, 2011, 115, 9651-9655.	1.5	30
45	Crystalâ€Sizeâ€Induced Band Gap Tuning in Perovskite Films. Angewandte Chemie - International Edition, 2021, 60, 21368-21376.	7.2	28
46	Intrinsic origin of two-dimensional electron gas at the (001) surface of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>SrTiO</mml:mtext><mml:mn>3</mml:mn></mml:msu Physical Review B, 2015, 91, .	1.1	27
47	Atomistic study of the interaction between a microcrack and a hard inclusion inÎ²â^'SiC. Physical Review B, 2004, 70, .	1.1	26
48	Layered Germanium Hybrid Perovskite Bromides: Insights from Experiments and Firstâ€Principles Calculations. Advanced Functional Materials, 2019, 29, 1903528.	7.8	26
49	Remarkably Weak Anisotropy in Thermal Conductivity of Two-Dimensional Hybrid Perovskite Butylammonium Lead Iodide Crystals. Nano Letters, 2021, 21, 3708-3714.	4.5	26
50	Machine-Learned Charge Transfer Integrals for Multiscale Simulations in Organic Thin Films. Journal of Physical Chemistry C, 2020, 124, 17733-17743.	1.5	25
51	Atomistic study of the dissolution of small boron interstitial clusters in c-Si. Applied Physics Letters, 2005, 87, 191912.	1.5	24
52	The dominant role of surfaces in the hysteretic behavior of hybrid perovskites. Nano Energy, 2020, 67, 104162.	8.2	24
53	Energetics of native point defects in cubic silicon carbide. European Physical Journal B, 2004, 38, 437-444.	0.6	22
54	Atomistic Simulations of P(NDI2OD-T2) Morphologies: From Single Chain to Condensed Phases. Journal of Physical Chemistry B, 2014, 118, 12556-12565.	1.2	22

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55	Competing Forces in the Self-Assembly of Coupled ZnO Nanopyramids. ACS Nano, 2015, 9, 3685-3694.	7.3	22
56	Atomistic fracture: QFM vs. MD. Engineering Fracture Mechanics, 2008, 75, 1794-1803.	2.0	20
57	Poly(3-hexylthiophene) Adhesion on Zinc Oxide Nanoneedles. Journal of Physical Chemistry C, 2011, 115, 16833-16837.	1.5	20
58	Thermally induced recrystallization of textured hydrogenated nanocrystalline silicon. Physical Review B, 2014, 89, .	1.1	20
59	Nonuniform Growth of Embedded Silicon Nanocrystals in an Amorphous Matrix. Physical Review Letters, 2007, 99, 205501.	2.9	19
60	The study of polythiophene/water interfaces by sum-frequency generation spectroscopy and molecular dynamics simulations. Journal of Materials Chemistry B, 2015, 3, 6429-6438.	2.9	19
61	Defect energetics of Î²-SiC using a new tight-binding molecular dynamics model. Journal of Nuclear Materials, 2004, 329-333, 1219-1222.	1.3	18
62	Crystallization kinetics of mixed amorphous-crystalline nanosystems. Physical Review B, 2008, 78, .	1.1	18
63	Mean-field theory for Josephson junction arrays with charge frustration. Physical Review B, 2000, 61, 11676-11688.	1.1	17
64	Fracture toughness of nanostructured silicon carbide. Applied Physics Letters, 2005, 87, 141912.	1.5	17
65	Lattice strain induced by boron clusters in crystalline silicon. Semiconductor Science and Technology, 2006, 21, L41-L44.	1.0	17
66	Electronic localization and optical absorption in embedded silicon nanograins. Applied Physics Letters, 2009, 94, 053115.	1.5	17
67	Electronic Properties and Quantum Confinement in Bi₂S₃ Ribbon-Like Nanostructures. Journal of Physical Chemistry C, 2013, 117, 21923-21929.	1.5	17
68	Linking morphology to thermal conductivity in PEDOT: an atomistic investigation. Journal Physics D: Applied Physics, 2017, 50, 494002.	1.3	17
69	Dielectric function of hybrid perovskites at finite temperature investigated by classical molecular dynamics. Journal of Chemical Physics, 2020, 152, 104705.	1.2	17
70	Ag/In leadâ€free double perovskites. EcoMat, 2020, 2, e12017.	6.8	16
71	Self-Assembled Lead Halide Perovskite Nanocrystals in a Perovskite Matrix. ACS Energy Letters, 2017, 2, 769-775.	8.8	15
72	Self-Assembling of Zinc Phthalocyanines on ZnO (101Ì…0) Surface through Multiple Time Scales. ACS Nano, 2011, 5, 9639-9647.	7.3	14

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73	Optoelectronic properties of (ZnO)60 isomers. Physical Chemistry Chemical Physics, 2012, 14, 14293.	1.3	14
74	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.	1.5	14
75	Failure strength of brittle materials containing nanovoids. Physical Review B, 2007, 75, .	1.1	13
76	Electronic Properties of Hybrid Zinc Oxideâ€“Oligothiophene Nanostructures. Journal of Physical Chemistry C, 2012, 116, 8174-8180.	1.5	13
77	Role of Molecular Thermodynamical Processes at Functionalized Polymer/Metaloxide Interfaces for Photovoltaics. Journal of Physical Chemistry C, 2013, 117, 13894-13901.	1.5	13
78	Atomistic Modeling of Morphology and Electronic Properties of Colloidal Ultrathin Bi₂S₃ Nanowires. Journal of Physical Chemistry C, 2015, 119, 16913-16919.	1.5	13
79	Kinetics and energeticsÂof metal halide perovskite conversion reactions at the nanoscale. Communications Materials, 2022, 3, .	2.9	12
80	Atomistic Investigation of the Solidâ€“Liquid Interface between the Crystalline Zinc Oxide Surface and the Liquid Tetrahydrofuran Solvent. Journal of Physical Chemistry C, 2012, 116, 12644-12648.	1.5	10
81	A (time-dependent) density functional theory study of the optoelectronic properties of bis-triisopropylsilylethynyl-functionalized acenes. Thin Solid Films, 2013, 543, 32-34.	0.8	10
82	Carrier Localization in Nanocrystalline Silicon. Journal of Physical Chemistry C, 2014, 118, 13417-13423.	1.5	10
83	Defect Dynamics in MAPbI₃ Polycrystalline Films: The Trapping Effect of Grain Boundaries. Helvetica Chimica Acta, 2020, 103, e2000110.	1.0	10
84	Crystalâ€Sizeâ€Induced Band Gap Tuning in Perovskite Films. Angewandte Chemie, 2021, 133, 21538-21546.	1.6	10
85	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.	1.0	9
86	Computational Materials Science application programming interface (CMSapi): a tool for developing applications for atomistic simulations. Computer Physics Communications, 2005, 169, 462-466.	3.0	9
87	Colloidal synthesis and characterization of Bi₂S₃nanoparticles for photovoltaic applications. Journal of Physics: Conference Series, 2014, 566, 012017.	0.3	9
88	Adhesion and Diffusion of Zinc-Phthalocyanines on the ZnO (101Ì…0) Surface. Journal of Physical Chemistry C, 2011, 115, 18208-18212.	1.5	8
89	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.	4.0	7
90	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.	8.2	7

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91	Long-lived electrets and lack of ferroelectricity in methylammonium lead bromide CH₃NH₃PbBr₃ ferroelastic single crystals. Physical Chemistry Chemical Physics, 2021, 23, 3233-3245.	1.3	7
92	On the solid-phase epitaxy of the a-Si:B/c-Si interface. Europhysics Letters, 2003, 62, 862-868.	0.7	6
93	Highly Emissive Layers based on Organic/Inorganic Nanohybrids Using Aggregation Induced Emission Effect. Advanced Materials Technologies, 2022, 7, 2100876.	3.0	6
94	Modeling of Self-Interstitial Diffusion in Implanted Molecular Beam Epitaxy Silicon. Materials Research Society Symposia Proceedings, 2002, 717, 1.	0.1	5
95	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.	2.7	5
96	Calculation of the local optoelectronic properties of nanostructured silicon. Physical Review B, 2009, 79, .	1.1	4
97	Pinpointing the Cause of Platinum Tipping on CdS Nanorods. Journal of Physical Chemistry C, 2015, 119, 22663-22668.	1.5	3
98	Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH₃NH₃PbI₃ Perovskites. Journal of Physical Chemistry C, 2019, 123, 6753-6762.	1.5	3
99	Simulations of Oxide/Polymer Hybrids. , 2015, , 1-13.		3
100	Boron ripening in amorphous silicon by large scale molecular dynamics simulations. Computational Materials Science, 2004, 30, 143-149.	1.4	2
101	Atomistic simulations of thiol-terminated modifiers for hybrid photovoltaic interfaces. Thin Solid Films, 2014, 560, 34-38.	0.8	1
102	Confinement of vibrational modes within crystalline lattices using thin amorphous layers. Journal of Physics Condensed Matter, 2017, 29, 145302.	0.7	1
103	Crack-tip stress shielding by a hard fiber in Î²-SiC: an atomistic study. Computer Physics Communications, 2005, 169, 40-43.	3.0	0
104	Simulations of Oxide/Polymer Hybrids. , 2016, , 3696-3707.		0
105	Bulk Structural and Electronic Properties at the Density Functional Theory and Post-Density Functional Theory Level of Calculation. , 2017, , 43-86.		0
106	Structure and Thermodynamic Properties of Hybrid Perovskites by Classical Molecular Dynamics. , 2017, , 1-42.		0