

Claudio Quarti

List of Publications by Year in descending order

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51
papers

4,472
citations

279778

23
h-index

243610

44
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52
all docs

52
docs citations

52
times ranked

6562
citing authors

#	ARTICLE	IF	CITATIONS
1	Cation-Induced Band-Gap Tuning in Organohalide Perovskites: Interplay of Spin-Orbit Coupling and Octahedra Tilting. <i>Nano Letters</i> , 2014, 14, 3608-3616.	9.1	1,033
2	The Raman Spectrum of the $\text{CH}_3\text{NH}_3\text{PbI}_3$ Hybrid Perovskite: Interplay of Theory and Experiment. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 279-284.	4.6	555
3	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.	30.8	423
4	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.	6.7	286
5	Phonon coherences reveal the polaronic character of excitons in two-dimensional lead halide perovskites. <i>Nature Materials</i> , 2019, 18, 349-356.	27.5	257
6	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, 3836-3842.	4.6	238
7	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, 16137-16144.	2.8	211
8	Photoinduced Reversible Structural Transformations in Free-Standing $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite Films. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2332-2338.	4.6	190
9	Ferroelectric Polarization of $\text{CH}_3\text{NH}_3\text{PbI}_3$: A Detailed Study Based on Density Functional Theory and Symmetry Mode Analysis. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2223-2231.	4.6	179
10	Influence of Surface Termination on the Energy Level Alignment at the $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite/C60 Interface. <i>Chemistry of Materials</i> , 2017, 29, 958-968.	6.7	149
11	Structural and electronic properties of organo-halide hybrid perovskites from ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9394-9409.	2.8	130
12	Formation of Long-Lived Color Centers for Broadband Visible Light Emission in Low-Dimensional Layered Perovskites. <i>Journal of the American Chemical Society</i> , 2017, 139, 18632-18639.	13.7	111
13	Tuning the Optoelectronic Properties of Two-Dimensional Hybrid Perovskite Semiconductors with Alkyl Chain Spacers. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3416-3424.	4.6	77
14	Ab Initio Calculation of the IR Spectrum of PTFE: Helical Symmetry and Defects. <i>Journal of Physical Chemistry B</i> , 2013, 117, 706-718.	2.6	60
15	Ab Initio Calculation of the Crystalline Structure and IR Spectrum of Polymers: Nylon 6 Polymorphs. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8299-8311.	2.6	56
16	Vibrational Response of Methylammonium Lead Iodide: From Cation Dynamics to Phonon-Phonon Interactions. <i>ChemSusChem</i> , 2016, 9, 2994-3004.	6.8	51
17	A computational investigation on singlet and triplet exciton couplings in acene molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18615.	2.8	44
18	Chlorine Incorporation in the $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite: Small Concentration, Big Effect. <i>Inorganic Chemistry</i> , 2017, 56, 74-83.	4.0	40

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19	Lead-Halide Perovskites Meet Donor-acceptor Charge-Transfer Complexes. <i>Chemistry of Materials</i> , 2019, 31, 6880-6888.	6.7	36
20	Fashioning Fluorous Organic Spacers for Tunable and Stable Layered Hybrid Perovskites. <i>Chemistry of Materials</i> , 2018, 30, 8211-8220.	6.7	35
21	IR spectroscopy of crystalline polymers from ab initio calculations: Nylon 6,6. <i>Vibrational Spectroscopy</i> , 2013, 66, 83-92.	2.2	32
22	Hot-Hole Cooling Controls the Initial Ultrafast Relaxation in Methylammonium Lead Iodide Perovskite. <i>Scientific Reports</i> , 2018, 8, 8115.	3.3	32
23	Physical properties of bulk, defective, 2D and 0D metal halide perovskite semiconductors from a symmetry perspective. <i>JPhys Materials</i> , 2020, 3, 042001.	4.2	29
24	Tetrazine molecules as an efficient electronic diversion channel in 2D organic-inorganic perovskites. <i>Materials Horizons</i> , 2021, 8, 1547-1560.	12.2	24
25	Electronic Structure and Optical Properties of Mixed Iodine/Bromine Lead Perovskites. To Mix or Not to Mix?. <i>Advanced Optical Materials</i> , 2021, 9, 2001832.	7.3	17
26	Cation Engineering for Resonant Energy Level Alignment in Two-Dimensional Lead Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2528-2535.	4.6	17
27	Stable 6H Organic-Inorganic Hybrid Lead Perovskite and Competitive Formation of 6H and 3C Perovskite Structure with Mixed A Cations. <i>ACS Applied Energy Materials</i> , 2019, 2, 5427-5437.	5.1	15
28	First principles modeling of exciton-polaritons in polydiacetylene chains. <i>Journal of Chemical Physics</i> , 2020, 153, 084103.	3.0	14
29	Fluorination of Organic Spacer Impacts on the Structural and Optical Response of 2D Perovskites. <i>Frontiers in Chemistry</i> , 2019, 7, 946.	3.6	14
30	Spatial Charge Separation as the Origin of Anomalous Stark Effect in Fluorous 2D Hybrid Perovskites. <i>Advanced Functional Materials</i> , 2020, 30, 2000228.	14.9	12
31	Organic Cations Protect Methylammonium Lead Iodide Perovskites against Small Exciton-Polaron Formation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2983-2991.	4.6	12
32	Revealing Weak Dimensional Confinement Effects in Excitonic Silver/Bismuth Double Perovskites. <i>Jacs Au</i> , 2022, 2, 136-149.	7.9	12
33	A density matrix based approach for studying excitons in organic crystals. <i>Chemical Physics Letters</i> , 2010, 496, 284-290.	2.6	11
34	Charge transfer complexes of a benzothienobenzothiophene derivative and their implementation as active layer in solution-processed thin film organic field-effect transistors. <i>Journal of Materials Chemistry C</i> , 2022, 10, 7319-7328.	5.5	11
35	Polymorphism of even nylons revisited through periodic quantum chemical calculations. <i>Polymer</i> , 2015, 67, 167-173.	3.8	10
36	Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4382-4391.	5.5	10

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37	Modelling Coupled Ion Motion in Electrolyte Solutions for Lithium-Sulfur Batteries. Batteries and Supercaps, 2019, 2, 473-481.	4.7	9
38	DFT Simulations as Valuable Tool to Support NMR Characterization of Halide Perovskites: the Case of Pure and Mixed Halide Perovskites. Helvetica Chimica Acta, 2021, 104, e2000231.	1.6	8
39	Light harvesting of CdSe/CdS quantum dots coated with β -cyclodextrin based host-guest species through resonant energy transfer from the guests. RSC Advances, 2014, 4, 28886-28892.	3.6	5
40	Nanoscale Studies at the Early Stage of Water-Induced Degradation of $\text{CH}_3\text{NH}_3\text{Pb}_3$ Perovskite Films Used for Photovoltaic Applications. ACS Applied Nano Materials, 2020, 3, 8268-8277.	5.0	5
41	A spectroscopic study of the optical properties of a nitrobenzoxadiazole derivative in solution: The role of specific interactions. Chemical Physics Letters, 2014, 610-611, 357-362.	2.6	3
42	Chapter 8. First Principles Modeling of Perovskite Solar Cells: Interplay of Structural, Electronic and Dynamical Effects. RSC Energy and Environment Series, 2016, , 234-296.	0.5	2
43	Synthesis and Characterization of $(\text{FA})_3(\text{HEA})_2\text{Pb}_3\text{I}_{11}$: A Rare Example of $\langle 110 \rangle$ -Oriented Multilayered Halide Perovskites. Chemistry of Materials, 2022, 34, 5780-5790.	6.7	2
44	Narrow and broadband light emission in layered organic lead halide perovskites: interplay between weak electron-lattice interactions and defect-related effects. , 2020, , .		1
45	Electric Properties of Organic-Inorganic Halide Perovskites and Their Role in the Working Principles of Perovskite-Based Solar Devices. , 2017, , 87-134.		0
46	Effect of electronically inert organic spacers on the optoelectronic properties of 2D hybrid perovskites. , 0, , .		0
47	Phonon coherences reveal the polaronic character of excitons in two-dimensional lead halide perovskites. , 0, , .		0
48	Electronic properties of 2D hybrid perovskites: spin-orbit coupling and indirect effect of inert organic spacers. , 0, , .		0
49	Effect of Electronically Inert Organic Spacers on the Optoelectronic Properties of 2D Hybrid Perovskites. , 0, , .		0
50	Framing excitons in halide perovskite materials from symmetry analysis and simulations. , 0, , .		0
51	Influence of Chemical Engineering, Photodoping and Lattice Distortions on the Optoelectronic Properties of Multilayered Perovskites. , 0, , .		0