

Claudio Quarti

List of Publications by Citations

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43
papers

3,641
citations

22
h-index

52
g-index

52
ext. papers

4,057
ext. citations

7.5
avg, IF

5.5
L-index

#	Paper	IF	Citations
43	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
42	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
41	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	15.4	355
40	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
39	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
38	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
37	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
36	Phonon coherences reveal the polaronic character of excitons in two-dimensional lead halide perovskites. <i>Nature Materials</i> , 2019 , 18, 349-356	27	160
35	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
34	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
33	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
32	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	16.4	90
31	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	6.4	55
30	Ab initio calculation of the IR spectrum of PTFE: helical symmetry and defects. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 706-18	3.4	53
29	Ab initio calculation of the crystalline structure and IR spectrum of polymers: nylon 6 polymorphs. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 8299-311	3.4	44
28	Vibrational Response of Methylammonium Lead Iodide: From Cation Dynamics to Phonon-Phonon Interactions. <i>ChemSusChem</i> , 2016 , 9, 2994-3004	8.3	38
27	Chlorine Incorporation in the CH ₃ NH ₃ PbI ₃ Perovskite: Small Concentration, Big Effect. <i>Inorganic Chemistry</i> , 2017 , 56, 74-83	5.1	36

26	A computational investigation on singlet and triplet exciton couplings in acene molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 18615-25	3.6	34
25	Fashioning Fluorous Organic Spacers for Tunable and Stable Layered Hybrid Perovskites. <i>Chemistry of Materials</i> , 2018 , 30, 8211-8220	9.6	27
24	Lead-Halide Perovskites Meet Donor-Acceptor Charge-Transfer Complexes. <i>Chemistry of Materials</i> , 2019 , 31, 6880-6888	9.6	26
23	Hot-Hole Cooling Controls the Initial Ultrafast Relaxation in Methylammonium Lead Iodide Perovskite. <i>Scientific Reports</i> , 2018 , 8, 8115	4.9	26
22	IR spectroscopy of crystalline polymers from ab initio calculations: Nylon 6,6. <i>Vibrational Spectroscopy</i> , 2013 , 66, 83-92	2.1	25
21	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	16
20	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	6.1	10
19	Fluorination of Organic Spacer Impacts on the Structural and Optical Response of 2D Perovskites. <i>Frontiers in Chemistry</i> , 2019 , 7, 946	5	9
18	Tetrazine molecules as an efficient electronic diversion channel in 2D organic-inorganic perovskites. <i>Materials Horizons</i> , 2021 , 8, 1547-1560	14.4	9
17	Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 4382-4391	7.1	8
16	A density matrix based approach for studying excitons in organic crystals. <i>Chemical Physics Letters</i> , 2010 , 496, 284-290	2.5	8
15	First principles modeling of exciton-polaritons in polydiacetylene chains. <i>Journal of Chemical Physics</i> , 2020 , 153, 084103	3.9	8
14	Modelling Coupled Ion Motion in Electrolyte Solutions for Lithium-Sulfur Batteries. <i>Batteries and Supercaps</i> , 2019 , 2, 473-481	5.6	8
13	Electronic Structure and Optical Properties of Mixed Iodine/Bromine Lead Perovskites. To Mix or Not to Mix?. <i>Advanced Optical Materials</i> , 2001832	8.1	8
12	Organic Cations Protect Methylammonium Lead Iodide Perovskites against Small Exciton-Polaron Formation. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 2983-2991	6.4	7
11	Polymorphism of even nylons revisited through periodic quantum chemical calculations. <i>Polymer</i> , 2015 , 67, 167-173	3.9	6
10	Spatial Charge Separation as the Origin of Anomalous Stark Effect in Fluorous 2D Hybrid Perovskites. <i>Advanced Functional Materials</i> , 2020 , 30, 2000228	15.6	6
9	DFT Simulations as Valuable Tool to Support NMR Characterization of Halide Perovskites: the Case of Pure and Mixed Halide Perovskites. <i>Helvetica Chimica Acta</i> , 2021 , 104, e2000231	2	5

8	Light harvesting of CdSe/CdS quantum dots coated with Cyclodextrin based host-guest species through resonant energy transfer from the guests. <i>RSC Advances</i> , 2014 , 4, 28886-28892	3.7	4
7	Cation Engineering for Resonant Energy Level Alignment in Two-Dimensional Lead Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 2528-2535	6.4	4
6	A spectroscopic study of the optical properties of a nitrobenzoxadiazole derivative in solution: The role of specific interactions. <i>Chemical Physics Letters</i> , 2014 , 610-611, 357-362	2.5	3
5	Chapter 8:First Principles Modeling of Perovskite Solar Cells: Interplay of Structural, Electronic and Dynamical Effects. <i>RSC Energy and Environment Series</i> , 2016 , 234-296	0.6	2
4	Nanoscale Studies at the Early Stage of Water-Induced Degradation of CH ₃ NH ₃ PbI ₃ Perovskite Films Used for Photovoltaic Applications. <i>ACS Applied Nano Materials</i> , 2020 , 3, 8268-8277	5.6	2
3	Revealing Weak Dimensional Confinement Effects in Excitonic Silver/Bismuth Double Perovskites.. <i>Jacs Au</i> , 2022 , 2, 136-149		2
2	Narrow and broadband light emission in layered organic lead halide perovskites: interplay between weak electron-lattice interactions and defect-related effects 2020 ,		1
1	Electric Properties of Organic-Inorganic Halide Perovskites and Their Role in the Working Principles of Perovskite-Based Solar Devices 2017 , 87-134		