Giacomo Giorgi

List of Publications by Citations

60 papers	2,139 citations	23 h-index	45 g-index
67 ext. papers	2,430 ext. citations	5.6 avg, IF	5.47 L-index

#	Paper	IF	Citations
60	Small Photocarrier Effective Masses Featuring Ambipolar Transport in Methylammonium Lead Iodide Perovskite: A Density Functional Analysis. *Journal of Physical Chemistry Letters*, **2013**, 4, 4213-6	6.4	543
59	Cation Role in Structural and Electronic Properties of 3D Organic–Inorganic Halide Perovskites: A DFT Analysis. *Journal of Physical Chemistry C*, **2014**, 118, 12176-12183	3.8	143
58	The mechanism of slow hot-hole cooling in lead-iodide perovskite: first-principles calculation on carrier lifetime from electron-phonon interaction. *Nano Letters*, **2015**, 15, 3103-8	11.5	121
57	Organic–Inorganic Hybrid Lead Iodide Perovskite Featuring Zero Dipole Moment Guanidinium Cations: A Theoretical Analysis. *Journal of Physical Chemistry C*, **2015**, 119, 4694-4701	3.8	108
56	Organic–inorganic halide perovskites: an ambipolar class of materials with enhanced photovoltaic performances. *Journal of Materials Chemistry A*, **2015**, 3, 8981-8991	13	89
55	Ice-Assisted Synthesis of Black Phosphorus Nanosheets as a Metal-Free Photocatalyst: 2D/2D Heterostructure for Broadband H2 Evolution. *Advanced Functional Materials*, **2019**, 29, 1902486	15.6	82
54	The Effects of the Organic-Inorganic Interactions on the Thermal Transport Properties of CH3NH3PbI3. *Nano Letters*, **2016**, 16, 2749-53	11.5	80
53	Penetration Barrier of Water through Graphynes' Pores: First-Principles Predictions and Force Field Optimization. *Journal of Physical Chemistry Letters*, **2014**, 5, 751-5	6.4	66
52	Graphdiyne Pores: "Ad Hoc" Openings for Helium Separation Applications. *Journal of Physical Chemistry C*, **2014**, 118, 29966-29972	3.8	61
51	Alternative, Lead-free, Hybrid Organic–Inorganic Perovskites for Solar Applications: A DFT Analysis. *Chemistry Letters*, **2015**, 44, 826-828	1.7	60
50	First principles investigation of hydrogen physical adsorption on graphynes' layers. *Carbon*, **2015**, 95, 1076-1081	10.4	50
49	Anion Ordering in CaTaO2N: Structural Impact on the Photocatalytic Activity. Insights from First-Principles. *Chemistry of Materials*, **2017**, 29, 539-545	9.6	44
48	Nonradical mechanisms for the uncatalyzed thermal functionalization of silicon surfaces by alkenes and alkynes: a density functional study. *Langmuir*, **2006**, 22, 9949-56	4	43
47	A Multitechnique Physicochemical Investigation of Various Factors Controlling the Photoaction Spectra and of Some Aspects of the Electron Transfer for a Series of Push–Pull Zn(II) Porphyrins Acting as Dyes in DSSCs. *Journal of Physical Chemistry C*, **2011**, 115, 23170-23182	3.8	41
46	Nature of the Electronic and Optical Excitations of Ruddlesden-Popper Hybrid Organic-Inorganic Perovskites: The Role of the Many-Body Interactions. *Journal of Physical Chemistry Letters*, **2018**, 9, 5891-5896	6.4	38
45	Zero-Dimensional Hybrid Organic-Inorganic Halide Perovskite Modeling: Insights from First Principles. *Journal of Physical Chemistry Letters*, **2016**, 7, 888-99	6.4	35
44	Optical Properties of Lead-Free Double Perovskites by Ab Initio Excited-State Methods. *ACS Energy Letters*, **2020**, 5, 457-463	20.1	34

43	A density functional tight binding study of acetic acid adsorption on crystalline and amorphous surfaces of titania. *Molecules*, **2015**, 20, 3371-88	4.8	33
42	Zero-dipole molecular organic cations in mixed organic-inorganic halide perovskites: possible chemical solution for the reported anomalous hysteresis in the current-voltage curve measurements. *Nanotechnology*, **2015**, 26, 442001	3.4	33
41	The Mechanism of Magnetic Interaction in Spin-Ladder Molecular Magnets: A First-Principles, Bottom-Up, Theoretical Study of the Magnetism in the Two-Legged Spin-Ladder Bis(2-amino-5-nitropyridinium) Tetrabromocuprate Monohydrate. *European Journal of Inorganic Chemistry*, **2005**, 2005, 4697-4706	2.3	31
40	A Novel Nanoporous Graphite Based on Graphynes: First-Principles Structure and Carbon Dioxide Preferential Physisorption. *ACS Applied Materials & Interfaces*, **2016**, 8, 27996-28003	9.5	27
39	First-principles study of fast Na diffusion in Na3P. *Chemical Physics Letters*, **2014**, 612, 129-133	2.5	24
38	DFT study of anatase-derived TiO2 nanosheets/graphene hybrid materials. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 1471-1479	1.3	23
37	The Nature of Radiative Transitions in TiO2-Based Nanosheets. *Journal of Physical Chemistry C*, **2012**, 116, 18495-18503	3.8	23
36	Excitons at the (001) surface of anatase: Spatial behavior and optical signatures. *Physical Review B*, **2011**, 84,	3.3	21
35	Lead-iodide nanowire perovskite with methylviologen showing interfacial charge-transfer absorption: a DFT analysis. *Physical Chemistry Chemical Physics*, **2014**, 16, 17955-9	3.6	20
34	Communication: Singularity-free hybrid functional with a Gaussian-attenuating exact exchange in a plane-wave basis. *Journal of Chemical Physics*, **2013**, 138, 241101	3.9	20
33	Two-dimensional optical excitations in the mixed-valence Cs2Au2I6 fully inorganic double perovskite. *Journal of Materials Chemistry C*, **2018**, 6, 10197-10201	7.1	20
32	Development of a Classical Interatomic Potential for MAPbBr3. *Journal of Physical Chemistry C*, **2017**, 121, 3724-3733	3.8	19
31	On the Chemical Origin of the Gap Bowing in (GaAs)(1-x)Ge(2x) Alloys: A Combined DFT-QSGW Study. *Nanoscale Research Letters*, **2010**, 5, 469-477	5	19
30	Role of Quantum-Confinement in Anatase Nanosheets. *Journal of Physical Chemistry Letters*, **2017**, 8, 3867-3873	6.4	17
29	Visible-to-Near-IR Wide-Range Light Harvesting by Interfacial Charge-Transfer Transitions between TiO2 and p-Aminophenol and Evidence of Direct Electron Injection to the Conduction Band of TiO2. *Journal of Physical Chemistry C*, **2017**, 121, 18710-18716	3.8	16
28	Structural and electronic features of small hybrid organic-inorganic halide perovskite clusters: a theoretical analysis. *Physical Chemistry Chemical Physics*, **2016**, 18, 27124-27132	3.6	13
27	Unraveling the adsorption mechanism of aromatic and aliphatic diols on the TiO2 surface: a density functional theory analysis. *Physical Chemistry Chemical Physics*, **2013**, 15, 9761-7	3.6	12
26	A density functional study on the Pt(0)-catalysed hydrosilylation of ethylene. *Computational and Theoretical Chemistry*, **2003**, 623, 277-288		11

25	MgTaO2N Photocatalysts: Perovskite versus Ilmenite Structure. A Theoretical Investigation. *Journal of Physical Chemistry C*, **2017**, 121, 27813-27821	3.8	10
24	Zirconium and hafnium oxide interface with silicon: Computational study of stress and strain effects. *Computational Materials Science*, **2008**, 43, 930-937	3.2	10
23	Strong out-of-plane excitons in 2D hybrid halide double perovskites. *Applied Physics Letters*, **2021**, 119, 051103	3.4	10
22	A Scalable Method for Thickness and Lateral Engineering of 2D Materials. *ACS Nano*, **2020**, 14, 4861-4870	16.7	8
21	Oxidative addition of SiH4 to Pt(PH3)2: a dynamical density functional study. *Chemical Physics Letters*, **2002**, 364, 87-92	2.5	8
20	Printable smart 3D architectures of regenerated silk on poly(3-hydroxybutyrate-co-3-hydroxyvalerate). *Materials and Design*, **2021**, 201, 109492	8.1	8
19	Effect of organic cation states on electronic properties of mixed organic-inorganic halide perovskite clusters. *Physical Chemistry Chemical Physics*, **2019**, 21, 8161-8169	3.6	7
18	First-principles investigation of the Lewis acid-base adduct formation at the methylammonium lead iodide surface. *Physical Chemistry Chemical Physics*, **2018**, 20, 11183-11195	3.6	7
17	Halide Pb-Free Double Perovskites: Ternary vs. Quaternary Stoichiometry. *Energies*, **2020**, 13, 3516	3.1	7
16	Carbon Nanotubes/Regenerated Silk Composite as a Three-Dimensional Printable Bio-Adhesive Ink with Self-Powering Properties. *ACS Applied Materials & Interfaces*, **2021**, 13, 21007-21017	9.5	7
15	Bridging the Fields of Solar Cell and Battery Research to Develop High-Performance Anodes for Photoelectrochemical Cells and Metal Ion Batteries. *Challenges*, **2013**, 4, 116-135	3.4	6
14	Materials Design and Optimization for Next-Generation Solar Cell and Light-Emitting Technologies. *Journal of Physical Chemistry Letters*, **2021**, 12, 4638-4657	6.4	5
13	A-site phase segregation in mixed cation perovskite. *Materials Reports Energy*, **2021**, 100064		4
12	Smart Parental Advisory: A Usage Control and Deep Learning-Based Framework for Dynamic Parental Control on Smart TV. *Lecture Notes in Computer Science*, **2017**, 118-133	0.9	4
11	Engineering Graphene Oxide/Water Interface from First Principles to Experiments for Electrostatic Protective Composites. *Polymers*, **2020**, 12,	4.5	4
10	Permeation of chemisorbed hydrogen through graphene: A flipping mechanism elucidated. *Carbon*, **2021**, 178, 718-727	10.4	4
9	Structural and electronic features of Si/CH3NH3PbI3 interfaces with optoelectronic applicability: Insights from first-principles. *Nano Energy*, **2020**, 67, 104166	17.1	3
8	Modeling of plasmonic properties of nanostructures for next generation solar cells and beyond. *Advances in Physics: X*, **2021**, 6, 1908848	5.1	2

List of Publications

7	Electronic and Optical Properties of Low-Dimensional TiO2: From Minority Surfaces to Nanocomposites. *ACS Symposium Series*, **2015**, 47-80	0.4	1
6	Doping of III–V Arsenide and Phosphide Wurtzite Semiconductors. *Journal of Physical Chemistry C*, **2020**, 124, 27203-27212	3.8	1
5	Theoretical Analysis on Mechanisms Implied in Hybrid Integrated Circuit Building. *Lecture Notes in Computer Science*, **2003**, 331-340	0.9	1
4	On the dual deuterium/deuteron nature of D charge distribution in the Ti host matrix: A DFT analysis. *International Journal of Hydrogen Energy*, **2013**, 38, 16477-16484	6.7	
3	Clustering and Octet Rule Violation Impact on Band Gap Bowing: Ab Initio Calculation of the Electronic Properties of (GaAs)1−(Ge2)xAlloys. *Chemistry Letters*, **2011**, 40, 770-772	1.7	
2	Advances in two-dimensional green materials for organic electronics applications **2022**, 391-422		
1	Electronic and Optical Properties of Nitrogen-Doped Layered Manganese Oxides. *Ceramic Transactions*,135-140	0.1	