

Paolo Umari

List of Publications by Citations

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24
papers

15,645
citations

15
h-index

27
g-index

27
ext. papers

18,257
ext. citations

5.3
avg, IF

5.71
L-index

#	Paper	IF	Citations
24	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , 2009 , 21, 395502	1.8	13251
23	Relativistic GW calculations on CH ₃ NH ₃ PbI ₃ and CH ₃ NH ₃ SnI ₃ perovskites for solar cell applications. <i>Scientific Reports</i> , 2014 , 4, 4467	4.9	910
22	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
21	Electronic and optical properties of mixed SnPb organohalide perovskites: a first principles investigation. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 9208-9215	13	156
20	Electronic and optical properties of MAPbX perovskites (X = I, Br, Cl): a unified DFT and GW theoretical analysis. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 27158-27164	3.6	108
19	Microscopic theory and quantum simulation of atomic heat transport. <i>Nature Physics</i> , 2016 , 12, 80-84	16.2	63
18	Infrared Dielectric Screening Determines the Low Exciton Binding Energy of Metal-Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 620-627	6.4	62
17	Chlorine Incorporation in the CH ₃ NH ₃ PbI Perovskite: Small Concentration, Big Effect. <i>Inorganic Chemistry</i> , 2017 , 56, 74-83	5.1	36
16	Photoelectron properties of DNA and RNA bases from many-body perturbation theory. <i>Physical Review B</i> , 2011 , 84,	3.3	32
15	Dielectric effect of a thin SiO ₂ interlayer at the interface between silicon and high-k oxides. <i>Microelectronic Engineering</i> , 2004 , 72, 299-303	2.5	24
14	Detailed analysis of plastic shear in the Raman spectra of SiO ₂ glass. <i>Journal of Non-Crystalline Solids</i> , 2015 , 428, 6-19	3.9	23
13	Large-scale GW-BSE calculations with N ³ scaling: Excitonic effects in dye-sensitized solar cells. <i>Physical Review B</i> , 2017 , 95,	3.3	22
12	Electronic structure of MAPbI and MAPbCl: importance of band alignment. <i>Scientific Reports</i> , 2019 , 9, 15159	4.9	21
11	First-principles investigation of organic photovoltaic materials C60, C70, [C60]PCBM, and bis-[C60]PCBM using a many-body G ₀ W ₀ -Lanczos approach. <i>Physical Review B</i> , 2015 , 91,	3.3	17
10	Surface susceptibility and conductivity of MoS ₂ and WSe ₂ monolayers: A first-principles and ellipsometry characterization. <i>Physical Review B</i> , 2020 , 101,	3.3	16
9	Dielectric susceptibility of dipolar molecular liquids by ab initio molecular dynamics: application to liquid HCl. <i>Chemical Physics Letters</i> , 2004 , 390, 193-198	2.5	15
8	Transition Dipole Moments of = 1, 2, and 3 Perovskite Quantum Wells from the Optical Stark Effect and Many-Body Perturbation Theory. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 716-723	6.4	14

7	Harnessing molecular excited states with Lanczos chains. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 074204	1.8	14
6	SIMPLE code: Optical properties with optimal basis functions. <i>Computer Physics Communications</i> , 2019 , 240, 106-119	4.2	11
5	Koopmans Meets Bethe-Salpeter: Excitonic Optical Spectra without GW. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3710-3720	6.4	9
4	Real Space-Real Time Evolution of Excitonic States Based on the Bethe-Salpeter Equation Method. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 7261-7269	6.4	2
3	Artificial photosynthesis: photoanodes based on polyquinoid dyes onto mesoporous tin oxide surface. <i>Photochemical and Photobiological Sciences</i> , 2021 , 20, 1243-1255	4.2	1
2	Accelerating GW Calculations with Optimal Polarizability Basis 2011 , 61-78		
1	The G W Method for Excited States Calculations 2021 , 483-495		