Paolo Umari

List of Publications by Year in Descending Order

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	Real Space-Real Time Evolution of Excitonic States Based on the Bethe-Salpeter Equation Method. *Journal of Physical Chemistry Letters*, **2021**, 12, 7261-7269	6.4	2
23	The G W Method for Excited States Calculations **2021**, 483-495		
22	Artificial photosynthesis: photoanodes based on polyquinoid dyes onto mesoporous tin oxide surface. *Photochemical and Photobiological Sciences*, **2021**, 20, 1243-1255	4.2	1
21	Transition Dipole Moments of = 1, 2, and 3 Perovskite Quantum Wells from the Optical Stark Effect and Many-Body Perturbation Theory. *Journal of Physical Chemistry Letters*, **2020**, 11, 716-723	6.4	14
20	Surface susceptibility and conductivity of MoS2 and WSe2 monolayers: A first-principles and ellipsometry characterization. *Physical Review B*, **2020**, 101,	3.3	16
19	Koopmans Meets Bethe-Salpeter: Excitonic Optical Spectra without GW. *Journal of Chemical Theory and Computation*, **2019**, 15, 3710-3720	6.4	9
18	SIMPLE code: Optical properties with optimal basis functions. *Computer Physics Communications*, **2019**, 240, 106-119	4.2	11
17	Electronic structure of MAPbI and MAPbCl: importance of band alignment. *Scientific Reports*, **2019**, 9, 15159	4.9	21
16	Infrared Dielectric Screening Determines the Low Exciton Binding Energy of Metal-Halide Perovskites. *Journal of Physical Chemistry Letters*, **2018**, 9, 620-627	6.4	62
15	Large-scale GW-BSE calculations with N3 scaling: Excitonic effects in dye-sensitized solar cells. *Physical Review B*, **2017**, 95,	3.3	22
14	Chlorine Incorporation in the CHNHPbI Perovskite: Small Concentration, Big Effect. *Inorganic Chemistry*, **2017**, 56, 74-83	5.1	36
13	Microscopic theory and quantum simulation of atomic heat transport. *Nature Physics*, **2016**, 12, 80-84	16.2	63
12	Electronic and optical properties of MAPbX perovskites (X = I, Br, Cl): a unified DFT and GW theoretical analysis. *Physical Chemistry Chemical Physics*, **2016**, 18, 27158-27164	3.6	108
11	First-principles investigation of organic photovoltaic materials C60, C70, [C60]PCBM, and bis-[C60]PCBM using a many-body G0W0-Lanczos approach. *Physical Review B*, **2015**, 91,	3.3	17
10	Detailed analysis of plastic shear in the Raman spectra of SiO2 glass. *Journal of Non-Crystalline Solids*, **2015**, 428, 6-19	3.9	23
9	Electronic and optical properties of mixed Sn-Pb organohalide perovskites: a first principles investigation. *Journal of Materials Chemistry A*, **2015**, 3, 9208-9215	13	156
8	Relativistic GW calculations on CH3NH3PbI3 and CH3NH3SnI3 perovskites for solar cell applications. *Scientific Reports*, **2014**, 4, 4467	4.9	910

List of Publications

7	Cation-induced band-gap tuning in organohalide perovskites: interplay of spin-orbit coupling and octahedra tilting. *Nano Letters*, **2014**, 14, 3608-16	11.5	837
6	Photoelectron properties of DNA and RNA bases from many-body perturbation theory. *Physical Review B*, **2011**, 84,	3.3	32
5	Accelerating GW Calculations with Optimal Polarizability Basis **2011**, 61-78		
4	Harnessing molecular excited states with Lanczos chains. *Journal of Physics Condensed Matter*, **2010** , 22, 074204	1.8	14
3	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, **2009**, 21, 395502	1.8	13251
2	Dielectric effect of a thin SiO2 interlayer at the interface between silicon and high-k oxides. *Microelectronic Engineering*, **2004**, 72, 299-303	2.5	24
1	Dielectric susceptibility of dipolar molecular liquids by ab initio molecular dynamics: application to liquid HCl. *Chemical Physics Letters*, **2004**, 390, 193-198	2.5	15