# Paolo Umari

List of Publications by Year
in descending order



| | | | |
|---|---|---|---|
| 25 papers | 21,189 citations | 430754 18 h-index | 610775 24 g-index |
| 27 all docs | 27 docs citations | 27 times ranked | 24525 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502. | 0.7 | 18,183 |
| 2 | Relativistic GW calculations on CH3NH3PbI3 and CH3NH3SnI3 Perovskites for Solar Cell Applications. Scientific Reports, 2014, 4, 4467. | 1.6 | 1,093 |
| 3 | Cation-Induced Band-Gap Tuning in Organohalide Perovskites: Interplay of Spinâ€“Orbit Coupling and Octahedra Tilting. Nano Letters, 2014, 14, 3608-3616. | 4.5 | 1,033 |
| 4 | Electronic and optical properties of mixed Snâ€“Pb organohalide perovskites: a first principles investigation. Journal of Materials Chemistry A, 2015, 3, 9208-9215. | 5.2 | 170 |
| 5 | Electronic and optical properties of MAPbX<sub>3</sub> perovskites (X = I, Br, Cl): a unified DFT and GW theoretical analysis. Physical Chemistry Chemical Physics, 2016, 18, 27158-27164. | 1.3 | 140 |
| 6 | Microscopic theory and quantum simulation of atomic heat transport. Nature Physics, 2016, 12, 80-84. | 6.5 | 93 |
| 7 | Infrared Dielectric Screening Determines the Low Exciton Binding Energy of Metal-Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 620-627. | 2.1 | 88 |
| 8 | Electronic structure of MAPbI3 and MAPbCl3: importance of band alignment. Scientific Reports, 2019, 9, 15159. | 1.6 | 52 |
| 9 | Chlorine Incorporation in the CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> Perovskite: Small Concentration, Big Effect. Inorganic Chemistry, 2017, 56, 74-83. | 1.9 | 40 |
| 10 | Large-scale <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m -BSE calculations with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>N</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:m scaling: Excitonic effects in dye-sensitized solar cells. Physical Review B, 2017, 95, . | 1.1 | 34 |
| 11 | Photoelectron properties of DNA and RNA bases from many-body perturbation theory. Physical Review B, 2011, 84, . | 1.1 | 32 |
| 12 | Detailed analysis of plastic shear in the Raman spectra of SiO2 glass. Journal of Non-Crystalline Solids, 2015, 428, 6-19. | 1.5 | 29 |
| 13 | Surface susceptibility and conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></ and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WSe</mml:mi><mml:mn>2</mml:mn></mml:msub></ monolayers: A first-principles and ellipsometry characterization. Physical Review B, 2020, 101, . | 1.1 | 28 |
| 14 | Dielectric effect of a thin SiO2 interlayer at the interface between silicon and high-k oxides. Microelectronic Engineering, 2004, 72, 299-303. | 1.1 | 26 |
| 15 | Dielectric susceptibility of dipolar molecular liquids by ab initio molecular dynamics: application to liquid HCl. Chemical Physics Letters, 2004, 390, 193-198. | 1.2 | 24 |
| 16 | Transition Dipole Moments of n = 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. | 2.1 | 24 |
| 17 | First-principles investigation of organic photovoltaic materials<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>C</mml:mtext><mml:mn>60</mml:mn></ml and bis-<mml:math xmlns:mml="h. Physical Review B, 2015, 91, . | 1.1 | 24 |
| 18 | SIMPLE code: Optical properties with optimal basis functions. Computer Physics Communications, 2019, 240, 106-119. | 3.0 | 21 |

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|---|---|---|---|
| 19 | Koopmans Meets Betheâ€“Salpeter: Excitonic Optical Spectra without GW. Journal of Chemical Theory and Computation, 2019, 15, 3710-3720. | 2.3 | 20 |
| 20 | Harnessing molecular excited states with Lanczos chains. Journal of Physics Condensed Matter, 2010, 22, 074204. | 0.7 | 15 |
| 21 | Artificial photosynthesis: photoanodes based on polyquinoid dyes onto mesoporous tin oxide surface. Photochemical and Photobiological Sciences, 2021, 20, 1243-1255. | 1.6 | 10 |
| 22 | Bethe-Salpeter equation approach with electron-phonon coupling for exciton binding energies. Physical Review B, 2021, 103, . | 1.1 | 9 |
| 23 | Real Spaceâ€“Real Time Evolution of Excitonic States Based on the Bethe-Salpeter Equation Method. Journal of Physical Chemistry Letters, 2021, 12, 7261-7269. | 2.1 | 2 |
| 24 | A Fully Linear Response G<sub>0</sub>W<sub>0</sub> Method That Scales Linearly up to Tens of Thousands of Cores. Journal of Physical Chemistry A, 2022, 126, 3384-3391. | 1.1 | 2 |
| 25 | Inclusion of infrared dielectric screening in the GW method from polaron energies to charge mobilities. Npj Computational Materials, 2022, 8, . | 3.5 | 0 |