Giovanni Di Liberto

List of Publications by Year
in descending order

41 papers	1,325 citations	279487 23 h-index	360668 35 g-index
41 all docs	41 docs citations	41 times ranked	847 citing authors

#	Article	IF	Citations
1	Density Functional Theory Estimate of Halide Perovskite Band Gap: When Spin Orbit Coupling Helps. Journal of Physical Chemistry C, 2022, 126, 2184-2198.	1.5	40
2	LaFeO₃ meets nitrogen-doped graphene functionalized with ultralow Pt loading in an impactful Z-scheme platform for photocatalytic hydrogen evolution. Journal of Materials Chemistry A, 2022, 10, 3330-3340.	5.2	14
3	Azide-Alkyne Click Chemistry over a Heterogeneous Copper-Based Single-Atom Catalyst. ACS Catalysis, 2022, 12, 2947-2958.	5.5	68
4	First principles approach to solar energy conversion efficiency of semiconductor heterojunctions. Solar Energy, 2022, 236, 445-454.	2.9	6
5	Interfacing single-atom catalysis with continuous-flow organic electrosynthesis. Chemical Society Reviews, 2022, 51, 3898-3925.	18.7	50
6	Universal Principles for the Rational Design of Single Atom Electrocatalysts? Handle with Care. ACS Catalysis, 2022, 12, 5846-5856.	5.5	60
7	pH Dependence of MgO, TiO₂, and Î³-Al₂O₃ Surface Chemistry from First Principles. Journal of Physical Chemistry C, 2022, 126, 10216-10223.	1.5	21
8	Z-Scheme versus type-II junction in g-C₃N₄/TiO₂ and g-C₃N₄/SrTiO₃/TiO₂ heterostructures. Catalysis Science and Technology, 2021, 11, 3589-3598.	2.1	25
9	Role of surface termination and quantum size in Î±-CsPbX₃ (X = Cl, Br, I) 2D nanostructures for solar light harvesting. Physical Chemistry Chemical Physics, 2021, 23, 3031-3040.	1.3	20
10	Plasmonic Au nanoclusters dispersed in nitrogen-doped graphene as a robust photocatalyst for light-to-hydrogen conversion. Journal of Materials Chemistry A, 2021, 9, 22810-22819.	5.2	26
11	Structural and electronic properties of TiO2 from first principles calculations. , 2021, , 67-85.		2
12	Direct measurement and modeling of spontaneous charge migration across anataseâ€“brookite nanoheterojunctions. Journal of Materials Chemistry A, 2021, 9, 7782-7790.	5.2	14
13	Nature and Role of Surface Junctions in BiOIO₃ Photocatalysts. Advanced Functional Materials, 2021, 31, 2009472.	7.8	20
14	Structure and Band Alignment of InP Photocatalysts Passivated by TiO₂ Thin Films. Journal of Physical Chemistry C, 2021, 125, 11620-11627.	1.5	7
15	Structures and properties of Pd nanoparticles intercalated in layered TiO2: A computational study. Catalysis Today, 2021, , .	2.2	1
16	Band offset in semiconductor heterojunctions. Journal of Physics Condensed Matter, 2021, 33, 415002.	0.7	19
17	WO₃/BiVO₄ Photoanodes: Facets Matching at the Heterojunction and BiVO₄ Layer Thickness Effects. ACS Applied Energy Materials, 2021, 4, 8421-8431.	2.5	22
18	Rational Design of Semiconductor Heterojunctions for Photocatalysis. Chemistry - A European Journal, 2021, 27, 13306-13317.	1.7	44

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19	Computational study of group III-V semiconductors and their interaction with oxide thin films. Solid-State Electronics, 2021, 184, 108038.	0.8	2
20	Role of surface termination in forming type-II photocatalyst heterojunctions: the case of TiO₂/BiVO₄. Journal of Physics Condensed Matter, 2021, 33, 075001.	0.7	18
21	Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts. Journal of the American Chemical Society, 2021, 143, 20431-20441.	6.6	77
22	Quantum confinement in group IIIâ€“V semiconductor 2D nanostructures. Nanoscale, 2020, 12, 17494-17501.	2.8	46
23	Nature of SrTiO3/TiO2 (anatase) heterostructure from hybrid density functional theory calculations. Journal of Chemical Physics, 2020, 152, 184704.	1.2	23
24	Band Gap in Magnetic Insulators from a Charge Transition Level Approach. Journal of Chemical Theory and Computation, 2020, 16, 3786-3798.	2.3	22
25	Charge Carriers Cascade in a Ternary TiO₂/TiO₂/ZnS Heterojunction: A DFT Study. ChemCatChem, 2020, 12, 2097-2105.	1.8	25
26	Theoretical treatment of semiconductor heterojunctions for photocatalysis: the WO₃/BiVO₄ interface. Journal of Physics Condensed Matter, 2019, 31, 434001.	0.7	16
27	Band Gap of 3D Metal Oxides and Quasi-2D Materials from Hybrid Density Functional Theory: Are Dielectric-Dependent Functionals Superior?. Journal of Chemical Theory and Computation, 2019, 15, 6294-6312.	2.3	45
28	Nitrogen doping in coexposed (001)â€“(101) anatase TiO₂ surfaces: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 21497-21505.	1.3	36
29	Reduced rovibrational coupling Cartesian dynamics for semiclassical calculations: Application to the spectrum of the Zundel cation. Journal of Chemical Physics, 2019, 151, 114307.	1.2	26
30	Vibrational investigation of nucleobases by means of divide and conquer semiclassical dynamics. Journal of Chemical Physics, 2019, 150, 224107.	1.2	29
31	Role of Heterojunction in Charge Carrier Separation in Coexposed Anatase (001)â€“(101) Surfaces. Journal of Physical Chemistry Letters, 2019, 10, 2372-2377.	2.1	46
32	â€œDivide and conquerâ€•semiclassical molecular dynamics: A practical method for spectroscopic calculations of high dimensional molecular systems. Journal of Chemical Physics, 2018, 148, 014307.	1.2	39
33	â€œDivide-and-conquerâ€•semiclassical molecular dynamics: An application to water clusters. Journal of Chemical Physics, 2018, 148, 104302.	1.2	38
34	A quantum mechanical insight into SN2 reactions: Semiclassical initial value representation calculations of vibrational features of the Clâ¯â‹¯CH3Cl pre-reaction complex with the VENUS suite of codes. Journal of Chemical Physics, 2018, 149, 164113.	1.2	19
35	Protonated glycine supramolecular systems: the need for quantum dynamics. Chemical Science, 2018, 9, 7894-7901.	3.7	35
36	A Close Look at the Structure of the TiO₂-APTES Interface in Hybrid Nanomaterials and Its Degradation Pathway: An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2017, 121, 430-440.	1.5	123

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37	Atomistic Explanation for Interlayer Charge Transfer in Metalâ€“Semiconductor Nanocomposites: The Case of Silver and Anatase. Journal of Physical Chemistry Letters, 2017, 8, 5372-5377.	2.1	25
38	Semiclassical â€œDivide-and-Conquerâ€•Method for Spectroscopic Calculations of High Dimensional Molecular Systems. Physical Review Letters, 2017, 119, 010401.	2.9	57
39	The importance of the pre-exponential factor in semiclassical molecular dynamics. Journal of Chemical Physics, 2016, 145, 144107.	1.2	36
40	Impregnation versus Bulk Synthesis: How the Synthetic Route Affects the Photocatalytic Efficiency of Nb/Ta:N Codoped TiO₂ Nanomaterials. Journal of Physical Chemistry C, 2015, 119, 24104-24115.	1.5	36
41	Unraveling the Cooperative Mechanism of Visible-Light Absorption in Bulk N,Nb Codoped TiO₂ Powders of Nanomaterials. Journal of Physical Chemistry C, 2014, 118, 24152-24164.	1.5	47