Giovanni Di Liberto

List of Publications by Year
in descending order

41 papers	1,325 citations	279798 23 h-index	361022 35 g-index
41 all docs	41 docs citations	41 times ranked	847 citing authors

#	Article	IF	Citations
1	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.	3.1	123
2	Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts. Journal of the American Chemical Society, 2021, 143, 20431-20441.	13.7	77
3	Azide-Alkyne Click Chemistry over a Heterogeneous Copper-Based Single-Atom Catalyst. ACS Catalysis, 2022, 12, 2947-2958.	11.2	68
4	Universal Principles for the Rational Design of Single Atom Electrocatalysts? Handle with Care. ACS Catalysis, 2022, 12, 5846-5856.	11.2	60
5	Semiclassical â€œDivide-and-Conquerâ€•Method for Spectroscopic Calculations of High Dimensional Molecular Systems. Physical Review Letters, 2017, 119, 010401.	7.8	57
6	Interfacing single-atom catalysis with continuous-flow organic electrosynthesis. Chemical Society Reviews, 2022, 51, 3898-3925.	38.1	50
7	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.	3.1	47
8	Role of Heterojunction in Charge Carrier Separation in Coexposed Anatase (001)â€“(101) Surfaces. Journal of Physical Chemistry Letters, 2019, 10, 2372-2377.	4.6	46
9	Quantum confinement in group IIIâ€“V semiconductor 2D nanostructures. Nanoscale, 2020, 12, 17494-17501.	5.6	46
10	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.	5.3	45
11	Rational Design of Semiconductor Heterojunctions for Photocatalysis. Chemistry - A European Journal, 2021, 27, 13306-13317.	3.3	44
12	Density Functional Theory Estimate of Halide Perovskite Band Gap: When Spin Orbit Coupling Helps. Journal of Physical Chemistry C, 2022, 126, 2184-2198.	3.1	40
13	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.	3.0	39
14	â€œDivide-and-conquerâ€•semiclassical molecular dynamics: An application to water clusters. Journal of Chemical Physics, 2018, 148, 104302.	3.0	38
15	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.	3.1	36
16	The importance of the pre-exponential factor in semiclassical molecular dynamics. Journal of Chemical Physics, 2016, 145, 144107.	3.0	36
17	Nitrogen doping in coexposed (001)â€“(101) anatase TiO₂ surfaces: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 21497-21505.	2.8	36
18	Protonated glycine supramolecular systems: the need for quantum dynamics. Chemical Science, 2018, 9, 7894-7901.	7.4	35

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19	Vibrational investigation of nucleobases by means of divide and conquer semiclassical dynamics. Journal of Chemical Physics, 2019, 150, 224107.	3.0	29
20	Reduced rovibrational coupling Cartesian dynamics for semiclassical calculations: Application to the spectrum of the Zundel cation. Journal of Chemical Physics, 2019, 151, 114307.	3.0	26
21	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.	10.3	26
22	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.	4.6	25
23	Charge Carriers Cascade in a Ternary TiO₂/TiO₂/ZnS Heterojunction: A DFT Study. ChemCatChem, 2020, 12, 2097-2105.	3.7	25
24	Z-Scheme versus type-II junction in g-C₃N₄/TiO₂ and g-C₃N₄/SrTiO₃/TiO₂ heterostructures. Catalysis Science and Technology, 2021, 11, 3589-3598.	4.1	25
25	Nature of SrTiO3/TiO2 (anatase) heterostructure from hybrid density functional theory calculations. Journal of Chemical Physics, 2020, 152, 184704.	3.0	23
26	Band Gap in Magnetic Insulators from a Charge Transition Level Approach. Journal of Chemical Theory and Computation, 2020, 16, 3786-3798.	5.3	22
27	WO₃/BiVO₄ Photoanodes: Facets Matching at the Heterojunction and BiVO₄ Layer Thickness Effects. ACS Applied Energy Materials, 2021, 4, 8421-8431.	5.1	22
28	pH Dependence of MgO, TiO₂, and Î³-Al₂O₃ Surface Chemistry from First Principles. Journal of Physical Chemistry C, 2022, 126, 10216-10223.	3.1	21
29	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.	2.8	20
30	Nature and Role of Surface Junctions in BiOIO₃ Photocatalysts. Advanced Functional Materials, 2021, 31, 2009472.	14.9	20
31	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.	3.0	19
32	Band offset in semiconductor heterojunctions. Journal of Physics Condensed Matter, 2021, 33, 415002.	1.8	19
33	Role of surface termination in forming type-II photocatalyst heterojunctions: the case of TiO₂/BiVO₄. Journal of Physics Condensed Matter, 2021, 33, 075001.	1.8	18
34	Theoretical treatment of semiconductor heterojunctions for photocatalysis: the WO₃/BiVO₄ interface. Journal of Physics Condensed Matter, 2019, 31, 434001.	1.8	16
35	Direct measurement and modeling of spontaneous charge migration across anataseâ€“brookite nanoheterojunctions. Journal of Materials Chemistry A, 2021, 9, 7782-7790.	10.3	14
36	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.	10.3	14

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37	Structure and Band Alignment of InP Photocatalysts Passivated by TiO₂ Thin Films. Journal of Physical Chemistry C, 2021, 125, 11620-11627.	3.1	7
38	First principles approach to solar energy conversion efficiency of semiconductor heterojunctions. Solar Energy, 2022, 236, 445-454.	6.1	6
39	Structural and electronic properties of TiO2 from first principles calculations. , 2021, , 67-85.		2
40	Computational study of group III-V semiconductors and their interaction with oxide thin films. Solid-State Electronics, 2021, 184, 108038.	1.4	2
41	Structures and properties of Pd nanoparticles intercalated in layered TiO2: A computational study. Catalysis Today, 2021, , .	4.4	1