

Giovanni Di Liberto

List of Publications by Year in descending order

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41
papers

1,325
citations

279487

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360668

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docs citations

41
times ranked

847
citing authors

#	ARTICLE	IF	CITATIONS
1	A Close Look at the Structure of the TiO ₂ -APTES Interface in Hybrid Nanomaterials and Its Degradation Pathway: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 430-440.	1.5	123
2	Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts. <i>Journal of the American Chemical Society</i> , 2021, 143, 20431-20441.	6.6	77
3	Azide-Alkyne Click Chemistry over a Heterogeneous Copper-Based Single-Atom Catalyst. <i>ACS Catalysis</i> , 2022, 12, 2947-2958.	5.5	68
4	Universal Principles for the Rational Design of Single Atom Electrocatalysts? Handle with Care. <i>ACS Catalysis</i> , 2022, 12, 5846-5856.	5.5	60
5	Semiclassical "Divide-and-Conquer" Method for Spectroscopic Calculations of High Dimensional Molecular Systems. <i>Physical Review Letters</i> , 2017, 119, 010401.	2.9	57
6	Interfacing single-atom catalysis with continuous-flow organic electrosynthesis. <i>Chemical Society Reviews</i> , 2022, 51, 3898-3925.	18.7	50
7	Unraveling the Cooperative Mechanism of Visible-Light Absorption in Bulk N,Nb Codoped TiO ₂ Powders of Nanomaterials. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24152-24164.	1.5	47
8	Role of Heterojunction in Charge Carrier Separation in Coexposed Anatase (001) " (101) Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2372-2377.	2.1	46
9	Quantum confinement in group III-V semiconductor 2D nanostructures. <i>Nanoscale</i> , 2020, 12, 17494-17501.	2.8	46
10	Band Gap of 3D Metal Oxides and Quasi-2D Materials from Hybrid Density Functional Theory: Are Dielectric-Dependent Functionals Superior?. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6294-6312.	2.3	45
11	Rational Design of Semiconductor Heterojunctions for Photocatalysis. <i>Chemistry - A European Journal</i> , 2021, 27, 13306-13317.	1.7	44
12	Density Functional Theory Estimate of Halide Perovskite Band Gap: When Spin Orbit Coupling Helps. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2184-2198.	1.5	40
13	"Divide and conquer" semiclassical molecular dynamics: A practical method for spectroscopic calculations of high dimensional molecular systems. <i>Journal of Chemical Physics</i> , 2018, 148, 014307.	1.2	39
14	"Divide-and-conquer" semiclassical molecular dynamics: An application to water clusters. <i>Journal of Chemical Physics</i> , 2018, 148, 104302.	1.2	38
15	Impregnation versus Bulk Synthesis: How the Synthetic Route Affects the Photocatalytic Efficiency of Nb/Ta:N Codoped TiO ₂ Nanomaterials. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24104-24115.	1.5	36
16	The importance of the pre-exponential factor in semiclassical molecular dynamics. <i>Journal of Chemical Physics</i> , 2016, 145, 144107.	1.2	36
17	Nitrogen doping in coexposed (001) " (101) anatase TiO ₂ surfaces: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21497-21505.	1.3	36
18	Protonated glycine supramolecular systems: the need for quantum dynamics. <i>Chemical Science</i> , 2018, 9, 7894-7901.	3.7	35

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19	Vibrational investigation of nucleobases by means of divide and conquer semiclassical dynamics. <i>Journal of Chemical Physics</i> , 2019, 150, 224107.	1.2	29
20	Reduced rovibrational coupling Cartesian dynamics for semiclassical calculations: Application to the spectrum of the Zundel cation. <i>Journal of Chemical Physics</i> , 2019, 151, 114307.	1.2	26
21	Plasmonic Au nanoclusters dispersed in nitrogen-doped graphene as a robust photocatalyst for light-to-hydrogen conversion. <i>Journal of Materials Chemistry A</i> , 2021, 9, 22810-22819.	5.2	26
22	Atomistic Explanation for Interlayer Charge Transfer in Metal-Semiconductor Nanocomposites: The Case of Silver and Anatase. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5372-5377.	2.1	25
23	Charge Carriers Cascade in a Ternary $\text{TiO}_2/\text{TiO}_2/\text{ZnS}$ Heterojunction: A DFT Study. <i>ChemCatChem</i> , 2020, 12, 2097-2105.	1.8	25
24	Z-Scheme <i>versus</i> type-II junction in $\text{g-C}_3\text{N}_4/\text{TiO}_2$ and $\text{g-C}_3\text{N}_4/\text{SrTiO}_3/\text{TiO}_2$ heterostructures. <i>Catalysis Science and Technology</i> , 2021, 11, 3589-3598.	2.1	25
25	Nature of $\text{SrTiO}_3/\text{TiO}_2$ (anatase) heterostructure from hybrid density functional theory calculations. <i>Journal of Chemical Physics</i> , 2020, 152, 184704.	1.2	23
26	Band Gap in Magnetic Insulators from a Charge Transition Level Approach. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3786-3798.	2.3	22
27	$\text{WO}_3/\text{BiVO}_4$ Photoanodes: Facets Matching at the Heterojunction and BiVO_4 Layer Thickness Effects. <i>ACS Applied Energy Materials</i> , 2021, 4, 8421-8431.	2.5	22
28	pH Dependence of MgO , TiO_2 , and Al_2O_3 Surface Chemistry from First Principles. <i>Journal of Physical Chemistry C</i> , 2022, 126, 10216-10223.	1.5	21
29	Role of surface termination and quantum size in CsPbX_3 ($X = \text{Cl}, \text{Br}, \text{I}$) 2D nanostructures for solar light harvesting. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3031-3040.	1.3	20
30	Nature and Role of Surface Junctions in BiOIO_3 Photocatalysts. <i>Advanced Functional Materials</i> , 2021, 31, 2009472.	7.8	20
31	A quantum mechanical insight into $\text{S}_\text{N}2$ reactions: Semiclassical initial value representation calculations of vibrational features of the $\text{Cl}^-\text{CH}_3\text{Cl}$ pre-reaction complex with the VENUS suite of codes. <i>Journal of Chemical Physics</i> , 2018, 149, 164113.	1.2	19
32	Band offset in semiconductor heterojunctions. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 415002.	0.7	19
33	Role of surface termination in forming type-II photocatalyst heterojunctions: the case of $\text{TiO}_2/\text{BiVO}_4$. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 075001.	0.7	18
34	Theoretical treatment of semiconductor heterojunctions for photocatalysis: the $\text{WO}_3/\text{BiVO}_4$ interface. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 434001.	0.7	16
35	Direct measurement and modeling of spontaneous charge migration across anatase-brookite nanoheterojunctions. <i>Journal of Materials Chemistry A</i> , 2021, 9, 7782-7790.	5.2	14
36	LaFeO_3 meets nitrogen-doped graphene functionalized with ultralow Pt loading in an impactful Z-scheme platform for photocatalytic hydrogen evolution. <i>Journal of Materials Chemistry A</i> , 2022, 10, 3330-3340.	5.2	14

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37	Structure and Band Alignment of InP Photocatalysts Passivated by TiO ₂ Thin Films. Journal of Physical Chemistry C, 2021, 125, 11620-11627.	1.5	7
38	First principles approach to solar energy conversion efficiency of semiconductor heterojunctions. Solar Energy, 2022, 236, 445-454.	2.9	6
39	Structural and electronic properties of TiO ₂ 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.	0.8	2
41	Structures and properties of Pd nanoparticles intercalated in layered TiO ₂ : A computational study. Catalysis Today, 2021, , .	2.2	1