

Cristiana Di Valentin

List of Publications by Year in descending order

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78
papers

5,704
citations

147801

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74163

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docs citations

78
times ranked

7630
citing authors

#	ARTICLE	IF	CITATIONS
1	Characterization of Paramagnetic Species in N-Doped TiO ₂ Powders by EPR Spectroscopy and DFT Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 11414-11419.	2.6	928
2	Theory of Carbon Doping of Titanium Dioxide. <i>Chemistry of Materials</i> , 2005, 17, 6656-6665.	6.7	663
3	Electronic Structure of Defect States in Hydroxylated and Reduced Rutile TiO ₂ (110) Surfaces. <i>Physical Review Letters</i> , 2006, 97, 166803.	7.8	592
4	Excess electron states in reduced bulk anatase TiO ₂ : Comparison of standard GGA, GGA+U, and hybrid DFT calculations. <i>Journal of Chemical Physics</i> , 2008, 129, 154113.	3.0	472
5	Theoretical Studies on Anatase and Less Common TiO ₂ Phases: Bulk, Surfaces, and Nanomaterials. <i>Chemical Reviews</i> , 2014, 114, 9708-9753.	47.7	367
6	Electronic and Structural Properties of WO ₃ : A Systematic Hybrid DFT Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8345-8353.	3.1	250
7	Bulk and Surface Polarons in Photoexcited Anatase TiO ₂ . <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2223-2228.	4.6	232
8	Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against structure calculations and experiments. <i>Physical Review B</i> , 2015, 91, .	3.2	140
9	Semiconductor-to-metal transition in WO ₃ : Nature of the oxygen vacancy. <i>Physical Review B</i> , 2011, 84, .	3.2	136
10	Water-Assisted Hole Trapping at the Highly Curved Surface of Nano-TiO ₂ Photocatalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 1415-1422.	13.7	95
11	Hole Scavenging by Organic Adsorbates on the TiO ₂ Surface: A DFT Model Study. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1901-1906.	4.6	93
12	Methanol on Anatase TiO ₂ (101): Mechanistic Insights into Photocatalysis. <i>ACS Catalysis</i> , 2017, 7, 7081-7091.	11.2	93
13	DFT Study of Hydrogen Adsorption On the Monoclinic WO ₃ (001) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10672-10679.	3.1	85
14	Operando visualization of the hydrogen evolution reaction with atomic-scale precision at different metal-graphene interfaces. <i>Nature Catalysis</i> , 2021, 4, 850-859.	34.4	81
15	H ₂ O Adsorption on WO ₃ and WO _{3-x} (001) Surfaces. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 23212-23221.	8.0	79
16	Band Gap in Magnetite above Verwey Temperature Induced by Symmetry Breaking. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25736-25742.	3.1	73
17	Anisotropic Effects of Oxygen Vacancies on Electrochromic Properties and Conductivity of β -Monoclinic WO ₃ . <i>Journal of Physical Chemistry C</i> , 2016, 120, 11716-11726.	3.1	70
18	Catalysis under Cover: Enhanced Reactivity at the Interface between (Doped) Graphene and Anatase TiO ₂ . <i>Journal of the American Chemical Society</i> , 2016, 138, 7365-7376.	13.7	69

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19	On-surface photo-dissociation of C-Br bonds: towards room temperature Ullmann coupling. <i>Chemical Communications</i> , 2015, 51, 12593-12596.	4.1	66
20	Accuracy of dielectric-dependent hybrid functionals in the prediction of optoelectronic properties of metal oxide semiconductors: a comprehensive comparison with many-body GW and experiments. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 044003.	1.8	59
21	Spherical versus Faceted Anatase TiO ₂ Nanoparticles: A Model Study of Structural and Electronic Properties. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20735-20746.	3.1	58
22	Copper single-atoms embedded in 2D graphitic carbon nitride for the CO ₂ reduction. <i>Npj 2D Materials and Applications</i> , 2021, 5, .	7.9	54
23	Single Atom Catalysts (SAC) trapped in defective and nitrogen-doped graphene supported on metal substrates. <i>Carbon</i> , 2021, 174, 772-788.	10.3	50
24	Modelling realistic TiO ₂ nanospheres: A benchmark study of SCC-DFTB against hybrid DFT. <i>Journal of Chemical Physics</i> , 2017, 147, 164701.	3.0	48
25	Water Multilayers on TiO ₂ (101) Anatase Surface: Assessment of a DFTB-Based Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3862-3873.	5.3	40
26	Anatase TiO ₂ Surface Functionalization by Alkylphosphonic Acid: A DFT+D Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2819-2828.	3.1	39
27	Charge Carriers Separation at the Graphene/(101) Anatase TiO ₂ Interface. <i>Advanced Materials Interfaces</i> , 2016, 3, 1500624.	3.7	37
28	Photoexcited carriers recombination and trapping in spherical vs faceted TiO ₂ nanoparticles. <i>Nano Energy</i> , 2016, 27, 673-689.	16.0	37
29	Curved TiO ₂ Nanoparticles in Water: Short (Chemical) and Long (Physical) Range Interfacial Effects. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 29943-29953.	8.0	35
30	Using Density Functional Theory to Model Realistic TiO ₂ Nanoparticles, Their Photoactivation and Interaction with Water. <i>Catalysts</i> , 2017, 7, 357.	3.5	34
31	Formaldehyde Adsorption on the Anatase TiO ₂ (101) Surface: Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8914-8922.	3.1	32
32	Impact of surface curvature, grafting density and solvent type on the PEGylation of titanium dioxide nanoparticles. <i>Journal of Colloid and Interface Science</i> , 2019, 555, 519-531.	9.4	32
33	Control of the Intermolecular Coupling of Dibromotetracene on Cu(110) by the Sequential Activation of C-Br and C-H Bonds. <i>Chemistry - A European Journal</i> , 2015, 21, 5826-5835.	3.3	30
34	Surface-Confined Polymerization of Halogenated Polyacenes: The Case of Dibromotetracene on Ag(110). <i>Journal of Physical Chemistry C</i> , 2016, 120, 4909-4918.	3.1	29
35	Optimizing PEGylation of TiO ₂ Nanocrystals through a Combined Experimental and Computational Study. <i>Chemistry of Materials</i> , 2019, 31, 7531-7546.	6.7	26
36	An efficient way to model complex magnetite: Assessment of SCC-DFTB against DFT. <i>Journal of Chemical Physics</i> , 2019, 150, 094703.	3.0	24

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37	Magnetic properties of nitrogen-doped ZrO ₂ : Theoretical evidence of absence of room temperature ferromagnetism. <i>Scientific Reports</i> , 2016, 6, 31435.	3.3	23
38	Bulk-terminated or reconstructed Fe ₃ O ₄ (001) surface: water makes a difference. <i>Nanoscale</i> , 2018, 10, 11021-11027.	5.6	23
39	Water at the Interface Between Defective Graphene and Cu or Pt (111) Surfaces. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 29932-29941.	8.0	22
40	Shaping Magnetite Nanoparticles from First Principles. <i>Physical Review Letters</i> , 2019, 123, 186101.	7.8	21
41	Synthesis of graphene nanoribbons with a defined mixed edge-site sequence by surface assisted polymerization of (1,6)-dibromopyrene on Ag(110). <i>Nanoscale</i> , 2016, 8, 17843-17853.	5.6	20
42	“Inside out” growth method for high-quality nitrogen-doped graphene. <i>Carbon</i> , 2021, 171, 704-710.	10.3	20
43	Nature of Paramagnetic Species in Nitrogen-Doped SnO ₂ : A Combined Electron Paramagnetic Resonance and Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26895-26903.	3.1	18
44	“Magnetism of Carbon Monovacancy in Graphene by Hybrid Density Functional Calculations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8653-8661.	3.1	17
45	Proton Transfers at a Dopamine-Functionalized TiO ₂ Interface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7682-7695.	3.1	17
46	Unraveling Dynamical and Light Effects on Functionalized Titanium Dioxide Nanoparticles for Bioconjugation. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10130-10144.	3.1	17
47	Oxygen reactivity on pure and B-doped graphene over crystalline Cu(111). Effects of the dopant and of the metal support. <i>Surface Science</i> , 2015, 634, 68-75.	1.9	16
48	Reactive molecular dynamics simulations of hydration shells surrounding spherical TiO ₂ nanoparticles: implications for proton-transfer reactions. <i>Nanoscale</i> , 2021, 13, 4151-4166.	5.6	16
49	Water on Graphene-Coated TiO ₂ : Role of Atomic Vacancies. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 5793-5804.	8.0	14
50	Insight into the interface between Fe ₃ O ₄ (001) surface and water overlayers through multiscale molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 124711.	3.0	14
51	Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO ₃ from First Principles. <i>ACS Catalysis</i> , 2019, 9, 10528-10535.	11.2	13
52	Computational Electrochemistry of Water Oxidation on Metal-Doped and Metal-Supported Defective h-BN. <i>ChemSusChem</i> , 2019, 12, 1995-2007.	6.8	12
53	Ab Initio Investigation of Polyethylene Glycol Coating of TiO ₂ Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 29190-29201.	3.1	11
54	Mechanism of CO Intercalation through the Graphene/Ni(111) Interface and Effect of Doping. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8887-8892.	4.6	11

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55	Nature of Excitons in Bidimensional WSe ₂ by Hybrid Density Functional Theory Calculations. <i>Nanomaterials</i> , 2018, 8, 481.	4.1	10
56	Gas Sensing by Metal and Nonmetal Co-Doped Graphene on a Ni Substrate. <i>Journal of Physical Chemistry C</i> , 2021, 125, 24079-24095.	3.1	10
57	Effect of dopamine-functionalization, charge and pH on protein corona formation around TiO ₂ nanoparticles. <i>Nanoscale</i> , 2022, 14, 5121-5137.	5.6	10
58	Interfacing CRYSTAL/AMBER to Optimize QM/MM Lennard-Jones Parameters for Water and to Study Solvation of TiO ₂ Nanoparticles. <i>Molecules</i> , 2018, 23, 2958.	3.8	9
59	Synthesis of corrugated C-based nanostructures by Br-corannulene oligomerization. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26161-26172.	2.8	9
60	Molecular dynamics simulations of doxorubicin in sphingomyelin-based lipid membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183763.	2.6	9
61	Pushing Down the Limit of NH ₃ Detection of Graphene-Based Chemiresistive Sensors through Functionalization by Thermally Activated Tetrazoles Dimerization. <i>ACS Nano</i> , 2022, 16, 10456-10469.	14.6	8
62	Molecular dynamics simulations of cRGD-conjugated PEGylated TiO ₂ nanoparticles for targeted photodynamic therapy. <i>Journal of Colloid and Interface Science</i> , 2022, 627, 126-141.	9.4	8
63	h-BN Defective Layers as Giant N-Donor Macrocycles for Cu Adatom Trapping from the Underlying Metal Substrate. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23610-23622.	3.1	7
64	Tuning graphene doping by carbon monoxide intercalation at the Ni(111) interface. <i>Carbon</i> , 2021, 176, 253-261.	10.3	7
65	Ab-Initio Spectroscopic Characterization of Melem-Based Graphitic Carbon Nitride Polymorphs. <i>Nanomaterials</i> , 2021, 11, 1863.	4.1	7
66	Can Single Metal Atoms Trapped in Defective h-BN/Cu(111) Improve Electrocatalysis of the H ₂ Evolution Reaction?. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23690-23698.	3.1	6
67	Dopamine-Decorated TiO ₂ Nanoparticles in Water: A QM/MM vs an MM Description. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6560-6574.	5.3	6
68	TETT-functionalized TiO ₂ nanoparticles for DOX loading: a quantum mechanical study at the atomic scale. <i>Nanoscale Advances</i> , 2020, 2, 2774-2784.	4.6	6
69	New Insights into Crystal Defects, Oxygen Vacancies, and Phase Transition of Ir-TiO ₂ . <i>Journal of Physical Chemistry C</i> , 2021, 125, 23548-23560.	3.1	6
70	Binding group of oligonucleotides on TiO ₂ surfaces: Phosphate anions or nucleobases?. <i>Applied Surface Science</i> , 2022, 575, 151560.	6.1	6
71	Rational design of nanosystems for simultaneous drug delivery and photodynamic therapy by quantum mechanical modeling. <i>Nanoscale</i> , 2019, 11, 15576-15588.	5.6	5
72	Multiscale simulations of the hydration shells surrounding spherical Fe ₃ O ₄ nanoparticles and effect on magnetic properties. <i>Nanoscale</i> , 2021, 13, 9293-9302.	5.6	5

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73	Using Coordination Chemistry Concepts to Unravel Electronic Properties of SACs in Bidimensional Materials. <i>Journal of Physical Chemistry C</i> , 2022, 126, 9615-9622.	3.1	5
74	Exploring the drug loading mechanism of photoactive inorganic nanocarriers through molecular dynamics simulations. <i>Nanoscale</i> , 2021, 13, 13000-13013.	5.6	4
75	Parametrization of the Fe-O-water cross-interaction for a more accurate Fe ₃ O ₄ /water interface model and its application to a spherical Fe ₃ O ₄ nanoparticle of realistic size. <i>Journal of Chemical Physics</i> , 2021, 154, 034702.	3.0	3
76	Tuning the electron injection mechanism by changing the adsorption mode: the case study of Alizarin on TiO ₂ . <i>Materials Today Energy</i> , 2022, 28, 101085.	4.7	3
77	Absorption mechanism of dopamine/DOPAC-modified TiO ₂ nanoparticles by time-dependent density functional theory calculations. <i>Materials Today Energy</i> , 2021, 19, 100571.	4.7	2
78	Insight into the Na adsorption on WSe ₂ /S ₂ (1-x) monolayers: a hybrid functional investigation. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 395001.	1.8	0