Cristiana Di Valentin

List of Publications by Year
in descending order

78	5,704	147566	74018
papers	citations	31 h-index	75 g-index

78	78	78	7630
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Characterization of Paramagnetic Species in N-Doped TiO2 Powders by EPR Spectroscopy and DFT Calculations. Journal of Physical Chemistry B, 2005, 109, 11414-11419.	1.2	928
2	Theory of Carbon Doping of Titanium Dioxide. Chemistry of Materials, 2005, 17, 6656-6665.	3.2	663
3	Electronic Structure of Defect States in Hydroxylated and Reduced RutileTiO2(110)Surfaces. Physical Review Letters, 2006, 97, 166803.	2.9	592
4	Excess electron states in reduced bulk anatase TiO2: Comparison of standard GGA, GGA+U, and hybrid DFT calculations. Journal of Chemical Physics, 2008, 129, 154113.	1.2	472
5	Theoretical Studies on Anatase and Less Common TiO₂ Phases: Bulk, Surfaces, and Nanomaterials. Chemical Reviews, 2014, 114, 9708-9753.	23.0	367
6	Electronic and Structural Properties of WO₃: A Systematic Hybrid DFT Study. Journal of Physical Chemistry C, 2011, 115, 8345-8353.	1.5	250
7	Bulk and Surface Polarons in Photoexcited Anatase TiO₂. Journal of Physical Chemistry Letters, 2011, 2, 2223-2228.	2.1	232
8	Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against<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 structure calculations and experiments. Physical Review B, 2015, 91, .	1.1	140
9	Semiconductor-to-metal transition in WO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn><mml:mo>â”</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>: Nature of the oxygen vacancy. Physical Review B, 2011, 84, .	1.1	136
10	Water-Assisted Hole Trapping at the Highly Curved Surface of Nano-TiO₂ Photocatalyst. Journal of the American Chemical Society, 2018, 140, 1415-1422.	6.6	95
11	Hole Scavenging by Organic Adsorbates on the TiO₂ Surface: A DFT Model Study. Journal of Physical Chemistry Letters, 2013, 4, 1901-1906.	2.1	93
12	Methanol on Anatase TiO₂ (101): Mechanistic Insights into Photocatalysis. ACS Catalysis, 2017, 7, 7081-7091.	5.5	93
13	DFT Study of Hydrogen Adsorption On the Monoclinic WO₃ (001) Surface. Journal of Physical Chemistry C, 2012, 116, 10672-10679.	1.5	85
14	Operando visualization of the hydrogen evolution reaction with atomic-scale precision at different metalâ€“graphene interfaces. Nature Catalysis, 2021, 4, 850-859.	16.1	81
15	H₂O Adsorption on WO₃ and WO_{3â€“x} (001) Surfaces. ACS Applied Materials & Interfaces, 2017, 9, 23212-23221.	4.0	79
16	Band Gap in Magnetite above Verwey Temperature Induced by Symmetry Breaking. Journal of Physical Chemistry C, 2017, 121, 25736-25742.	1.5	73
17	Anisotropic Effects of Oxygen Vacancies on Electrochromic Properties and Conductivity of Î³-Monoclinic WO₃. Journal of Physical Chemistry C, 2016, 120, 11716-11726.	1.5	70
18	Catalysis under Cover: Enhanced Reactivity at the Interface between (Doped) Graphene and Anatase TiO₂. Journal of the American Chemical Society, 2016, 138, 7365-7376.	6.6	69

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19	On-surface photo-dissociation of Câ€“Br bonds: towards room temperature Ullmann coupling. Chemical Communications, 2015, 51, 12593-12596.	2.2	66
20	Accuracy of dielectric-dependent hybrid functionals in the prediction of optoelectronic properties of metal oxide semiconductors: a comprehensive comparison with many-bodyGWand experiments. Journal of Physics Condensed Matter, 2018, 30, 044003.	0.7	59
21	Spherical versus Faceted Anatase TiO₂ Nanoparticles: A Model Study of Structural and Electronic Properties. Journal of Physical Chemistry C, 2015, 119, 20735-20746.	1.5	58
22	Copper single-atoms embedded in 2D graphitic carbon nitride for the CO2 reduction. Npj 2D Materials and Applications, 2021, 5, .	3.9	54
23	Single Atom Catalysts (SAC) trapped in defective and nitrogen-doped graphene supported on metal substrates. Carbon, 2021, 174, 772-788.	5.4	50
24	Modelling realistic TiO2 nanospheres: A benchmark study of SCC-DFTB against hybrid DFT. Journal of Chemical Physics, 2017, 147, 164701.	1.2	48
25	Water Multilayers on TiO₂ (101) Anatase Surface: Assessment of a DFTB-Based Method. Journal of Chemical Theory and Computation, 2017, 13, 3862-3873.	2.3	40
26	Anatase TiO₂ Surface Functionalization by Alkylphosphonic Acid: A DFT+D Study. Journal of Physical Chemistry C, 2012, 116, 2819-2828.	1.5	39
27	Charge Carriers Separation at the Graphene/(101) Anatase TiO₂ Interface. Advanced Materials Interfaces, 2016, 3, 1500624.	1.9	37
28	Photoexcited carriers recombination and trapping in spherical vs faceted TiO2 nanoparticles. Nano Energy, 2016, 27, 673-689.	8.2	37
29	Curved TiO₂ Nanoparticles in Water: Short (Chemical) and Long (Physical) Range Interfacial Effects. ACS Applied Materials & Interfaces, 2018, 10, 29943-29953.	4.0	35
30	Using Density Functional Theory to Model Realistic TiO2 Nanoparticles, Their Photoactivation and Interaction with Water. Catalysts, 2017, 7, 357.	1.6	34
31	Formaldehyde Adsorption on the Anatase TiO₂(101) Surface: Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2017, 121, 8914-8922.	1.5	32
32	Impact of surface curvature, grafting density and solvent type on the PEGylation of titanium dioxide nanoparticles. Journal of Colloid and Interface Science, 2019, 555, 519-531.	5.0	32
33	Control of the Intermolecular Coupling of Dibromotetracene on Cu(110) by the Sequential Activation of Cï£¿Br and Cï£¿H Bonds. Chemistry - A European Journal, 2015, 21, 5826-5835.	1.7	30
34	Surface-Confined Polymerization of Halogenated Polyacenes: The Case of Dibromotetracene on Ag(110). Journal of Physical Chemistry C, 2016, 120, 4909-4918.	1.5	29
35	Optimizing PEGylation of TiO₂ Nanocrystals through a Combined Experimental and Computational Study. Chemistry of Materials, 2019, 31, 7531-7546.	3.2	26
36	An efficient way to model complex magnetite: Assessment of SCC-DFTB against DFT. Journal of Chemical Physics, 2019, 150, 094703.	1.2	24

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37	Magnetic properties of nitrogen-doped ZrO2: Theoretical evidence of absence of room temperature ferromagnetism. Scientific Reports, 2016, 6, 31435.	1.6	23
38	Bulk-terminated or reconstructed Fe₃O₄(001) surface: water makes a difference. Nanoscale, 2018, 10, 11021-11027.	2.8	23
39	Water at the Interface Between Defective Graphene and Cu or Pt (111) Surfaces. ACS Applied Materials & Interfaces, 2017, 9, 29932-29941.	4.0	22
40	Shaping Magnetite Nanoparticles from First Principles. Physical Review Letters, 2019, 123, 186101.	2.9	21
41	Synthesis of graphene nanoribbons with a defined mixed edge-site sequence by surface assisted polymerization of (1,6)-dibromopyrene on Ag(110). Nanoscale, 2016, 8, 17843-17853.	2.8	20
42	â€œInside outâ€•growth method for high-quality nitrogen-doped graphene. Carbon, 2021, 171, 704-710.	5.4	20
43	Nature of Paramagnetic Species in Nitrogen-Doped SnO₂: A Combined Electron Paramagnetic Resonance and Density Functional Theory Study. Journal of Physical Chemistry C, 2015, 119, 26895-26903.	1.5	18
44	Ï€ Magnetism of Carbon Monovacancy in Graphene by Hybrid Density Functional Calculations. Journal of Physical Chemistry C, 2017, 121, 8653-8661.	1.5	17
45	Proton Transfers at a Dopamine-Functionalized TiO₂ Interface. Journal of Physical Chemistry C, 2019, 123, 7682-7695.	1.5	17
46	Unraveling Dynamical and Light Effects on Functionalized Titanium Dioxide Nanoparticles for Bioconjugation. Journal of Physical Chemistry C, 2019, 123, 10130-10144.	1.5	17
47	Oxygen reactivity on pure and B-doped graphene over crystalline Cu(111). Effects of the dopant and of the metal support. Surface Science, 2015, 634, 68-75.	0.8	16
48	Reactive molecular dynamics simulations of hydration shells surrounding spherical TiO₂nanoparticles: implications for proton-transfer reactions. Nanoscale, 2021, 13, 4151-4166.	2.8	16
49	Water on Graphene-Coated TiO2: Role of Atomic Vacancies. ACS Applied Materials & Interfaces, 2018, 10, 5793-5804.	4.0	14
50	Insight into the interface between Fe3O4 (001) surface and water overlayers through multiscale molecular dynamics simulations. Journal of Chemical Physics, 2020, 152, 124711.	1.2	14
51	Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO₃ from First Principles. ACS Catalysis, 2019, 9, 10528-10535.	5.5	13
52	Computational Electrochemistry of Water Oxidation on Metalâ€Doped and Metalâ€Supported Defective hâ€BN. ChemSusChem, 2019, 12, 1995-2007.	3.6	12
53	Ab Initio Investigation of Polyethylene Glycol Coating of TiO₂ Surfaces. Journal of Physical Chemistry C, 2016, 120, 29190-29201.	1.5	11
54	Mechanism of CO Intercalation through the Graphene/Ni(111) Interface and Effect of Doping. Journal of Physical Chemistry Letters, 2020, 11, 8887-8892.	2.1	11

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55	Nature of Excitons in Bidimensional WSe2 by Hybrid Density Functional Theory Calculations. Nanomaterials, 2018, 8, 481.	1.9	10
56	Gas Sensing by Metal and Nonmetal Co-Doped Graphene on a Ni Substrate. Journal of Physical Chemistry C, 2021, 125, 24079-24095.	1.5	10
57	Effect of dopamine-functionalization, charge and pH on protein corona formation around TiO₂ nanoparticles. Nanoscale, 2022, 14, 5121-5137.	2.8	10
58	Interfacing CRYSTAL/AMBER to Optimize QM/MM Lennardâ€"Jones Parameters for Water and to Study Solvation of TiO2 Nanoparticles. Molecules, 2018, 23, 2958.	1.7	9
59	Synthesis of corrugated C-based nanostructures by Br-corannulene oligomerization. Physical Chemistry Chemical Physics, 2018, 20, 26161-26172.	1.3	9
60	Molecular dynamics simulations of doxorubicin in sphingomyelin-based lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183763.	1.4	9
61	Pushing Down the Limit of NH₃ Detection of Graphene-Based Chemiresistive Sensors through Functionalization by Thermally Activated Tetrazoles Dimerization. ACS Nano, 2022, 16, 10456-10469.	7.3	8
62	Molecular dynamics simulations of cRGD-conjugated PEGylated TiO2 nanoparticles for targeted photodynamic therapy. Journal of Colloid and Interface Science, 2022, 627, 126-141.	5.0	8
63	h-BN Defective Layers as Giant N-Donor Macrocycles for Cu Adatom Trapping from the Underlying Metal Substrate. Journal of Physical Chemistry C, 2018, 122, 23610-23622.	1.5	7
64	Tuning graphene doping by carbon monoxide intercalation at the Ni(111) interface. Carbon, 2021, 176, 253-261.	5.4	7
65	Ab-Initio Spectroscopic Characterization of Melem-Based Graphitic Carbon Nitride Polymorphs. Nanomaterials, 2021, 11, 1863.	1.9	7
66	Can Single Metal Atoms Trapped in Defective h-BN/Cu(111) Improve Electrocatalysis of the H₂ Evolution Reaction?. Journal of Physical Chemistry C, 2020, 124, 23690-23698.	1.5	6
67	Dopamine-Decorated TiO₂ Nanoparticles in Water: A QM/MM vs an MM Description. Journal of Chemical Theory and Computation, 2020, 16, 6560-6574.	2.3	6
68	TETT-functionalized TiO2 nanoparticles for DOX loading: a quantum mechanical study at the atomic scale. Nanoscale Advances, 2020, 2, 2774-2784.	2.2	6
69	New Insights into Crystal Defects, Oxygen Vacancies, and Phase Transition of Ir-TiO2. Journal of Physical Chemistry C, 2021, 125, 23548-23560.	1.5	6
70	Binding group of oligonucleotides on TiO2 surfaces: Phosphate anions or nucleobases?. Applied Surface Science, 2022, 575, 151560.	3.1	6
71	Rational design of nanosystems for simultaneous drug delivery and photodynamic therapy by quantum mechanical modeling. Nanoscale, 2019, 11, 15576-15588.	2.8	5
72	Multiscale simulations of the hydration shells surrounding spherical Fe₃O₄nanoparticles and effect on magnetic properties. Nanoscale, 2021, 13, 9293-9302.	2.8	5

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73	Using Coordination Chemistry Concepts to Unravel Electronic Properties of SACs in Bidimensional Materials. Journal of Physical Chemistry C, 2022, 126, 9615-9622.	1.5	5
74	Exploring the drug loading mechanism of photoactive inorganic nanocarriers through molecular dynamics simulations. Nanoscale, 2021, 13, 13000-13013.	2.8	4
75	Parametrization of the Feâ€“Owater cross-interaction for a more accurate Fe3O4/water interface model and its application to a spherical Fe3O4 nanoparticle of realistic size. Journal of Chemical Physics, 2021, 154, 034702.	1.2	3
76	Tuning the electron injection mechanism by changing the adsorption mode: the case study of Alizarin on TiO2. Materials Today Energy, 2022, 28, 101085.	2.5	3
77	Absorption mechanism of dopamine/DOPAC-modified TiO2 nanoparticles by time-dependent density functional theory calculations. Materials Today Energy, 2021, 19, 100571.	2.5	2
78	Insight into the Na adsorption on WSe_{2x}S_{2(1â^’x)} monolayers: a hybrid functional investigation. Journal of Physics Condensed Matter, 2020, 32, 395001.	0.7	0