

# Cristiana Di Valentin

## List of Publications by Year in descending order

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Version: 2024-02-01

78  
papers

5,704  
citations

147566

31  
h-index

74018

75  
g-index

78  
all docs

78  
docs citations

78  
times ranked

7630  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular dynamics simulations of doxorubicin in sphingomyelin-based lipid membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183763.	1.4	9
2	Binding group of oligonucleotides on TiO <sub>2</sub> surfaces: Phosphate anions or nucleobases?. <i>Applied Surface Science</i> , 2022, 575, 151560.	3.1	6
3	Effect of dopamine-functionalization, charge and pH on protein corona formation around TiO <sub>2</sub> nanoparticles. <i>Nanoscale</i> , 2022, 14, 5121-5137.	2.8	10
4	Using Coordination Chemistry Concepts to Unravel Electronic Properties of SACs in Bidimensional Materials. <i>Journal of Physical Chemistry C</i> , 2022, 126, 9615-9622.	1.5	5
5	Pushing Down the Limit of NH <sub>3</sub> Detection of Graphene-Based Chemiresistive Sensors through Functionalization by Thermally Activated Tetrazoles Dimerization. <i>ACS Nano</i> , 2022, 16, 10456-10469.	7.3	8
6	Tuning the electron injection mechanism by changing the adsorption mode: the case study of Alizarin on TiO <sub>2</sub> . <i>Materials Today Energy</i> , 2022, 28, 101085.	2.5	3
7	Molecular dynamics simulations of cRGD-conjugated PEGylated TiO <sub>2</sub> nanoparticles for targeted photodynamic therapy. <i>Journal of Colloid and Interface Science</i> , 2022, 627, 126-141.	5.0	8
8	“Inside out” growth method for high-quality nitrogen-doped graphene. <i>Carbon</i> , 2021, 171, 704-710.	5.4	20
9	Single Atom Catalysts (SAC) trapped in defective and nitrogen-doped graphene supported on metal substrates. <i>Carbon</i> , 2021, 174, 772-788.	5.4	50
10	Absorption mechanism of dopamine/DOPAC-modified TiO <sub>2</sub> nanoparticles by time-dependent density functional theory calculations. <i>Materials Today Energy</i> , 2021, 19, 100571.	2.5	2
11	Multiscale simulations of the hydration shells surrounding spherical Fe <sub>3</sub> O <sub>4</sub> nanoparticles and effect on magnetic properties. <i>Nanoscale</i> , 2021, 13, 9293-9302.	2.8	5
12	Exploring the drug loading mechanism of photoactive inorganic nanocarriers through molecular dynamics simulations. <i>Nanoscale</i> , 2021, 13, 13000-13013.	2.8	4
13	Tuning graphene doping by carbon monoxide intercalation at the Ni(111) interface. <i>Carbon</i> , 2021, 176, 253-261.	5.4	7
14	Copper single-atoms embedded in 2D graphitic carbon nitride for the CO <sub>2</sub> reduction. <i>Npj 2D Materials and Applications</i> , 2021, 5, .	3.9	54
15	Ab-Initio Spectroscopic Characterization of Melem-Based Graphitic Carbon Nitride Polymorphs. <i>Nanomaterials</i> , 2021, 11, 1863.	1.9	7
16	Parametrization of the Fe–Owater cross-interaction for a more accurate Fe <sub>3</sub> O <sub>4</sub> /water interface model and its application to a spherical Fe <sub>3</sub> O <sub>4</sub> nanoparticle of realistic size. <i>Journal of Chemical Physics</i> , 2021, 154, 034702.	1.2	3
17	Reactive molecular dynamics simulations of hydration shells surrounding spherical TiO <sub>2</sub> nanoparticles: implications for proton-transfer reactions. <i>Nanoscale</i> , 2021, 13, 4151-4166.	2.8	16
18	Operando visualization of the hydrogen evolution reaction with atomic-scale precision at different metal–graphene interfaces. <i>Nature Catalysis</i> , 2021, 4, 850-859.	16.1	81

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19	New Insights into Crystal Defects, Oxygen Vacancies, and Phase Transition of Ir-TiO <sub>2</sub> . Journal of Physical Chemistry C, 2021, 125, 23548-23560.	1.5	6
20	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
21	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
22	Can Single Metal Atoms Trapped in Defective h-BN/Cu(111) Improve Electrocatalysis of the H <sub>2</sub> Evolution Reaction?. Journal of Physical Chemistry C, 2020, 124, 23690-23698.	1.5	6
23	Dopamine-Decorated TiO <sub>2</sub> Nanoparticles in Water: A QM/MM vs an MM Description. Journal of Chemical Theory and Computation, 2020, 16, 6560-6574.	2.3	6
24	Insight into the Na adsorption on WSe <sub>2</sub> S <sub>2</sub> (1 $\times$ 1 $\times$ ) monolayers: a hybrid functional investigation. Journal of Physics Condensed Matter, 2020, 32, 395001.	0.7	0
25	Insight into the interface between Fe <sub>3</sub> O <sub>4</sub> (001) surface and water overlayers through multiscale molecular dynamics simulations. Journal of Chemical Physics, 2020, 152, 124711.	1.2	14
26	TETT-functionalized TiO <sub>2</sub> nanoparticles for DOX loading: a quantum mechanical study at the atomic scale. Nanoscale Advances, 2020, 2, 2774-2784.	2.2	6
27	Proton Transfers at a Dopamine-Functionalized TiO <sub>2</sub> Interface. Journal of Physical Chemistry C, 2019, 123, 7682-7695.	1.5	17
28	Optimizing PEGylation of TiO <sub>2</sub> Nanocrystals through a Combined Experimental and Computational Study. Chemistry of Materials, 2019, 31, 7531-7546.	3.2	26
29	Rational design of nanosystems for simultaneous drug delivery and photodynamic therapy by quantum mechanical modeling. Nanoscale, 2019, 11, 15576-15588.	2.8	5
30	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
31	Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO <sub>3</sub> from First Principles. ACS Catalysis, 2019, 9, 10528-10535.	5.5	13
32	Shaping Magnetite Nanoparticles from First Principles. Physical Review Letters, 2019, 123, 186101.	2.9	21
33	Unraveling Dynamical and Light Effects on Functionalized Titanium Dioxide Nanoparticles for Bioconjugation. Journal of Physical Chemistry C, 2019, 123, 10130-10144.	1.5	17
34	An efficient way to model complex magnetite: Assessment of SCC-DFTB against DFT. Journal of Chemical Physics, 2019, 150, 094703.	1.2	24
35	Computational Electrochemistry of Water Oxidation on Metal-Doped and Metal-Supported Defective h-BN. ChemSusChem, 2019, 12, 1995-2007.	3.6	12
36	Water on Graphene-Coated TiO <sub>2</sub> : Role of Atomic Vacancies. ACS Applied Materials & Interfaces, 2018, 10, 5793-5804.	4.0	14

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37	Water-Assisted Hole Trapping at the Highly Curved Surface of Nano-TiO <sub>2</sub> Photocatalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 1415-1422.	6.6	95
38	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.	0.7	59
39	Interfacing CRYSTAL/AMBER to Optimize QM/MM Lennard-Jones Parameters for Water and to Study Solvation of TiO <sub>2</sub> Nanoparticles. <i>Molecules</i> , 2018, 23, 2958.	1.7	9
40	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.	1.5	7
41	Synthesis of corrugated C-based nanostructures by Br-corannulene oligomerization. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26161-26172.	1.3	9
42	Bulk-terminated or reconstructed Fe <sub>3</sub> O <sub>4</sub> (001) surface: water makes a difference. <i>Nanoscale</i> , 2018, 10, 11021-11027.	2.8	23
43	Curved TiO <sub>2</sub> Nanoparticles in Water: Short (Chemical) and Long (Physical) Range Interfacial Effects. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 29943-29953.	4.0	35
44	Nature of Excitons in Bidimensional WSe <sub>2</sub> by Hybrid Density Functional Theory Calculations. <i>Nanomaterials</i> , 2018, 8, 481.	1.9	10
45	Formaldehyde Adsorption on the Anatase TiO <sub>2</sub> (101) Surface: Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8914-8922.	1.5	32
46	H <sub>2</sub> O Adsorption on WO <sub>3</sub> and WO <sub>3</sub> ·xH <sub>2</sub> O (001) Surfaces. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 23212-23221.	4.0	79
47	Ï€ Magnetism of Carbon Monovacancy in Graphene by Hybrid Density Functional Calculations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8653-8661.	1.5	17
48	Band Gap in Magnetite above Verwey Temperature Induced by Symmetry Breaking. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25736-25742.	1.5	73
49	Methanol on Anatase TiO <sub>2</sub> (101): Mechanistic Insights into Photocatalysis. <i>ACS Catalysis</i> , 2017, 7, 7081-7091.	5.5	93
50	Water at the Interface Between Defective Graphene and Cu or Pt (111) Surfaces. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 29932-29941.	4.0	22
51	Modelling realistic TiO <sub>2</sub> nanospheres: A benchmark study of SCC-DFTB against hybrid DFT. <i>Journal of Chemical Physics</i> , 2017, 147, 164701.	1.2	48
52	Water Multilayers on TiO <sub>2</sub> (101) Anatase Surface: Assessment of a DFTB-Based Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3862-3873.	2.3	40
53	Using Density Functional Theory to Model Realistic TiO <sub>2</sub> Nanoparticles, Their Photoactivation and Interaction with Water. <i>Catalysts</i> , 2017, 7, 357.	1.6	34
54	Charge Carriers Separation at the Graphene/(101) Anatase TiO <sub>2</sub> Interface. <i>Advanced Materials Interfaces</i> , 2016, 3, 1500624.	1.9	37

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55	Magnetic properties of nitrogen-doped ZrO <sub>2</sub> : Theoretical evidence of absence of room temperature ferromagnetism. <i>Scientific Reports</i> , 2016, 6, 31435.	1.6	23
56	Anisotropic Effects of Oxygen Vacancies on Electrochromic Properties and Conductivity of $\beta$ -Monoclinic WO <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , 2016, 120, 11716-11726.	1.5	70
57	Catalysis under Cover: Enhanced Reactivity at the Interface between (Doped) Graphene and Anatase TiO <sub>2</sub> . <i>Journal of the American Chemical Society</i> , 2016, 138, 7365-7376.	6.6	69
58	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.	2.8	20
59	Photoexcited carriers recombination and trapping in spherical vs faceted TiO <sub>2</sub> nanoparticles. <i>Nano Energy</i> , 2016, 27, 673-689.	8.2	37
60	Ab Initio Investigation of Polyethylene Glycol Coating of TiO <sub>2</sub> Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 29190-29201.	1.5	11
61	Surface-Confined Polymerization of Halogenated Polyacenes: The Case of Dibromotetracene on Ag(110). <i>Journal of Physical Chemistry C</i> , 2016, 120, 4909-4918.	1.5	29
62	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.	1.7	30
63	Nature of Paramagnetic Species in Nitrogen-Doped SnO <sub>2</sub> : A Combined Electron Paramagnetic Resonance and Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26895-26903.	1.5	18
64	On-surface photo-dissociation of C-Br bonds: towards room temperature Ullmann coupling. <i>Chemical Communications</i> , 2015, 51, 12593-12596.	2.2	66
65	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, .	1.1	140
66	Spherical versus Faceted Anatase TiO <sub>2</sub> Nanoparticles: A Model Study of Structural and Electronic Properties. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20735-20746.	1.5	58
67	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.	0.8	16
68	Theoretical Studies on Anatase and Less Common TiO <sub>2</sub> Phases: Bulk, Surfaces, and Nanomaterials. <i>Chemical Reviews</i> , 2014, 114, 9708-9753.	23.0	367
69	Hole Scavenging by Organic Adsorbates on the TiO <sub>2</sub> Surface: A DFT Model Study. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1901-1906.	2.1	93
70	Anatase TiO <sub>2</sub> Surface Functionalization by Alkylphosphonic Acid: A DFT+D Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2819-2828.	1.5	39
71	DFT Study of Hydrogen Adsorption On the Monoclinic WO <sub>3</sub> (001) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10672-10679.	1.5	85
72	Electronic and Structural Properties of WO <sub>3</sub> : A Systematic Hybrid DFT Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8345-8353.	1.5	250

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73	Semiconductor-to-metal transition in $\text{WO}_3$ : Nature of the oxygen vacancy. Physical Review B, 2011, 84, .	1.1	136
74	Bulk and Surface Polarons in Photoexcited Anatase $\text{TiO}_2$ . Journal of Physical Chemistry Letters, 2011, 2, 2223-2228.	2.1	232
75	Excess electron states in reduced bulk anatase $\text{TiO}_2$ : Comparison of standard GGA, GGA+U, and hybrid DFT calculations. Journal of Chemical Physics, 2008, 129, 154113.	1.2	472
76	Electronic Structure of Defect States in Hydroxylated and Reduced Rutile $\text{TiO}_2(110)$ Surfaces. Physical Review Letters, 2006, 97, 166803.	2.9	592
77	Characterization of Paramagnetic Species in N-Doped $\text{TiO}_2$ Powders by EPR Spectroscopy and DFT Calculations. Journal of Physical Chemistry B, 2005, 109, 11414-11419.	1.2	928
78	Theory of Carbon Doping of Titanium Dioxide. Chemistry of Materials, 2005, 17, 6656-6665.	3.2	663