Gilberto Teobaldi

List of Publications by Year
in descending order

77 papers	3,254 citations	201674 27 h-index	149698 56 g-index
79 all docs	79 docs citations	79 times ranked	4429 citing authors

#	Article	IF	Citations
1	Macroscopic transport by synthetic molecular machines. Nature Materials, 2005, 4, 704-710.	27.5	685
2	Electron traps and their effect on the surface chemistry of TiO ₂ (110). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 2391-2396.	7.1	264
3	A Generic Basis for Some Simple Light-Operated Mechanical Molecular Machines. Journal of the American Chemical Society, 2004, 126, 12210-12211.	13.7	199
4	Beating the Stoner criterion using molecular interfaces. Nature, 2015, 524, 69-73.	27.8	151
5	Kinetics of Place-Exchange Reactions of Thiols on Gold Nanoparticles. Langmuir, 2003, 19, 5172-5174.	3.5	119
6	Extremely Strong and Readily Accessible AAAâ˜DDD Triple Hydrogen Bond Complexes. Journal of the American Chemical Society, 2007, 129, 476-477.	13.7	103
7	Cadiotâ€“Chodkiewicz Active Template Synthesis of Rotaxanes and Switchable Molecular Shuttles with Weak Intercomponent Interactions. Angewandte Chemie - International Edition, 2008, 47, 4392-4396.	13.8	101
8	The <scp>ONETEP</scp> linear-scaling density functional theory program. Journal of Chemical Physics, 2020, 152, 174111.	3.0	94
9	Geometric Structure ofTiO2(011)(2Ã—1). Physical Review Letters, 2008, 101, 185501.	7.8	87
10	The oxygen vacancy in Li-ion battery cathode materials. Nanoscale Horizons, 2020, 5, 1453-1466.	8.0	77
11	Spin-polarized electron transfer in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mtext>ferromagnet</mml:mtext></mml:mrow><mml:mo>/ Physical Review B, 2014, 90, .	3.2	59
12	Detection of catalytic intermediates at an electrode surface during carbon dioxide reduction by an earth-abundant catalyst. Nature Catalysis, 2018, 1, 952-959.	34.4	59
13	Modeling the Adsorption of Alkanes on an Au(111) Surface. Langmuir, 2003, 19, 7335-7340.	3.5	57
14	Density functional theory screening of gas-treatment strategies for stabilization of high energy-density lithium metal anodes. Journal of Power Sources, 2015, 296, 150-161.	7.8	57
15	Chemical Resolution at Ionic Crystal Surfaces Using Dynamic Atomic Force Microscopy with Metallic Tips. Physical Review Letters, 2011, 106, 216102.	7.8	56
16	Molecular Dynamics of a Dendrimerâ˜Dye Guestâ˜Host System. Journal of the American Chemical Society, 2003, 125, 7388-7393.	13.7	53
17	Modelling STM images of TiO2(110) from first-principles: Defects, water adsorption and dissociation products. Chemical Physics Letters, 2007, 437, 73-78.	2.6	52
18	Ab-initio calculations and STM observations on tetrapyridyl and Fe(II)-tetrapyridyl-porphyrin molecules on Ag(111). Surface Science, 2007, 601, 2409-2414.	1.9	46

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19	Work Function Evolution in Li Anode Processing. Advanced Energy Materials, 2020, 10, 2000520.	19.5	40
20	Scanning Tunneling Microscopy Contrast Mechanisms for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 109, 156105.	7.8	38
21	Recent advances in low-dimensional Janus materials: theoretical and simulation perspectives. Materials Advances, 2021, 2, 7543-7558.	5.4	38
22	The effect of van der Waals interactions on the properties of intrinsic defects in graphite. Carbon, 2010, 48, 4145-4161.	10.3	37
23	Amorphous Domains in Black Titanium Dioxide. Advanced Materials, 2021, 33, e2100407.	21.0	36
24	Modelling of the Adsorption of C60 on the Au(110) Surface. ChemPhysChem, 2004, 5, 245-248.	2.1	33
25	Structural resolution of inorganic nanotubes with complex stoichiometry. Nature Communications, 2018, 9, 2033.	12.8	33
26	(Sub)surface-Promoted Disproportionation and Absolute Band Alignment in High-Power LiMn₂O₄ Cathodes. Journal of Physical Chemistry C, 2015, 119, 21358-21368.	3.1	29
27	Chemically Selective Alternatives to Photoferroelectrics for Polarizationâ€Enhanced Photocatalysis: The Untapped Potential of Hybrid Inorganic Nanotubes. Advanced Science, 2017, 4, 1600153.	11.2	29
28	The potential of imogolite nanotubes as (co-)photocatalysts: a linear-scaling density functional theory study. Journal of Physics Condensed Matter, 2016, 28, 074003.	1.8	28
29	Structure and Oxygen Evolution Activity of Î²-NiOOH: Where Are the Protons?. ACS Catalysis, 2022, 12, 295-304.	11.2	28
30	Including the probe tip in theoretical models of inelastic scanning tunneling spectroscopy: CO on Cu(100). Physical Review B, 2007, 76, .	3.2	27
31	Variation in surface energy and reduction drive of a metal oxide lithium-ion anode with stoichiometry: a DFT study of lithium titanate spinel surfaces. Journal of Materials Chemistry A, 2016, 4, 17180-17192.	10.3	23
32	Adsorption of Organic Molecules on Gold Electrodes. Journal of Physical Chemistry C, 2007, 111, 13879-13885.	3.1	22
33	Hydroxyl vacancies in single-walled aluminosilicate and aluminogermanate nanotubes. Journal of Physics Condensed Matter, 2009, 21, 195301.	1.8	20
34	Emergent magnetism at transition-metalâ€“nanocarbon interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 5583-5588.	7.1	20
35	C₆₀ on Gold: Adsorption, Motion, and Viscosity. Small, 2007, 3, 1694-1698.	10.0	19
36	Optimization of constrained density functional theory. Physical Review B, 2016, 94, .	3.2	19

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37	Role of applied bias and tip electronic structure in the scanning tunneling microscopy imaging of highly oriented pyrolytic graphite. Physical Review B, 2012, 85, .	3.2	18
38	What is the orientation of the tip in a scanning tunneling microscope?. Progress in Surface Science, 2015, 90, 223-238.	8.3	18
39	Supercell convergence of charge-transfer energies in pentacene molecular crystals from constrained DFT. Physical Review B, 2016, 93, .	3.2	18
40	The Role of Cation-Vacancies for the Electronic and Optical Properties of Aluminosilicate Imogolite Nanotubes: A Non-local, Linear-Response TDDFT Study. Frontiers in Chemistry, 2019, 7, 210.	3.6	18
41	The unique carrier mobility of Janus MoSSe/GaN heterostructures. Frontiers of Physics, 2021, 16, 1.	5.0	18
42	Adsorption of benzene, fluorobenzene and metaâ€diâ€fluorobenzene on Cu(110): A computational study. Journal of Computational Chemistry, 2008, 29, 1589-1595.	3.3	17
43	Structure and properties of surface and subsurface defects in graphite accounting for van der Waals and spin-polarization effects. Physical Review B, 2010, 82, .	3.2	17
44	Large-scale density functional theory simulation of inorganic nanotubes: a case study on Imogolite nanotubes. Materials Research Innovations, 2015, 19, S272-S282.	2.3	17
45	Solid wetting-layers in inorganic nano-reactors: the water in imogolite nanotube case. Nanoscale Advances, 2020, 2, 1869-1877.	4.6	17
46	Creating pseudo-Kondo resonances by field-induced diffusion of atomic hydrogen. Nanotechnology, 2008, 19, 305701.	2.6	16
47	Internal Dynamics and Energy Transfer in Dansylated POPAM Dendrimers and Their Eosin Complexes. Journal of Physical Chemistry B, 2010, 114, 1548-1558.	2.6	15
48	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï€</mml:mi></mml:math> -anisotropy: A nanocarbon route to hard magnetism. Physical Review B, 2020, 101, .	3.2	15
49	Quantitative Resolution of Complex Stoichiometric Changes during Electrochemical Cycling by Density Functional Theory-Assisted Electrochemical Quartz Crystal Microbalance. ACS Applied Energy Materials, 2020, 3, 3347-3357.	5.1	14
50	Activity and selectivity of CO₂ photoreduction on catalytic materials. Dalton Transactions, 2020, 49, 12918-12928.	3.3	13
51	The Combined Role of Faceting and Heteroatom Doping for Hydrogen Evolution on a WC Electrocatalyst in Aqueous Solution: A Density Functional Theory Study. Journal of Physical Chemistry C, 2021, 125, 4602-4613.	3.1	13
52	Water-Hydrogen-Polaron Coupling at Anatase TiO2(101) Surfaces: A Hybrid Density Functional Theory Study. Journal of Physical Chemistry Letters, 2020, 11, 4317-4325.	4.6	12
53	Self-assembly of semifluorinated n-alkanethiols on {111}-oriented Au investigated with scanning tunneling microscopy experiment and theory. Journal of Chemical Physics, 2007, 127, 024702.	3.0	11
54	The role of permanent and induced electrostatic dipole moments for Schottky barriers in Janus MXY/graphene heterostructures: a first-principles study. Dalton Transactions, 0, , .	3.3	11

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55	Inapplicability of exact constraints and a minimal two-parameter generalization to the DFT+ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> based correction of self-interaction error. Physical Review B, 2016, 94, .	3.2	10
56	Reversible spin storage in metal oxideâ€"fullerene heterojunctions. Science Advances, 2020, 6, eaax1085.	10.3	10
57	Enhanced Spinâ€"Orbit Coupling in Heavy Metals via Molecular Coupling. ACS Applied Materials & Interfaces, 2021, 13, 5228-5234.	8.0	10
58	The effect of temperature on the internal dynamics of dansylated POPAM dendrimers. RSC Advances, 2011, 1, 1778.	3.6	9
59	Simulation of some dynamical aspects of the photophysics of dye molecules encapsulated in a dendrimer. Journal of Luminescence, 2005, 111, 335-342.	3.1	8
60	Contrast stability and â€˜stripeâ€™ formation in scanning tunnelling microscopy imaging of highly oriented pyrolytic graphite: the role of STM-tip orientations. Journal of Physics Condensed Matter, 2014, 26, 485007.	1.8	8
61	The unique carrier mobility of monolayer Janus MoSSe nanoribbons: a first-principles study. Dalton Transactions, 2021, 50, 10252-10260.	3.3	8
62	Termination Effects in Aluminosilicate and Aluminogermanate Imogolite Nanotubes: A Density Functional Theory Study. Crystals, 2020, 10, 1051.	2.2	6
63	Nonadiabatic Dynamics of Polaron Hopping and Coupling with Water on Reduced TiO₂. Journal of Physical Chemistry Letters, 2022, 13, 857-863.	4.6	6
64	The role of isotropic and anisotropic Hubbard corrections for the magnetic ordering and absolute band alignment of hematite Î±-Fe2O3(0001) surfaces. Progress in Natural Science: Materials International, 2019, 29, 349-355.	4.4	5
65	Effect of crystal field on the formation and diffusion of oxygen vacancy at anatase (101) surface and sub-surface. Progress in Natural Science: Materials International, 2020, 30, 128-133.	4.4	5
66	The Role of Thermal Fluctuations and Vibrational Entropy: A Theoretical Insight into the Î´-to-Î± Transition of FAPbI₃. Journal of Physical Chemistry Letters, 2022, 13, 3089-3095.	4.6	5
67	Understanding the Cosolvation Effect of Dendrimers. Journal of Chemical Theory and Computation, 2005, 1, 194-200.	5.3	4
68	Role of Metal Lattice Expansion and Molecular Ï€-Conjugation for the Magnetic Hardening at Cuâ€"Organics Interfaces. Journal of Physical Chemistry C, 2017, 121, 23777-23787.	3.1	4
69	Subspace Occupancy-Constraining Potentials for Modeling Polaron Formation. Journal of Physical Chemistry C, 2021, 125, 26354-26362.	3.1	4
70	Polymorphism and isomerisation of an azobenzene derivative on gold. Chemical Communications, 2011, 47, 8662.	4.1	3
71	Kinetic Monte Carlo modeling of oxide thin film growth. Journal of Chemical Physics, 2022, 156, .	3.0	3
72	Detection of spin-states in Mn-doped gallium arsenide films. Nanotechnology, 2007, 18, 044006.	2.6	1

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73	Theory of Scanning Tunneling Microscopy and Applications in Catalysis. , 0, , 97-118.		1
74	Combined Role of Biaxial Strain and Nonstoichiometry for the Electronic, Magnetic, and Redox Properties of Lithiated Metal-Oxide Films: The LiMn₂O₄ Case. ACS Applied Materials & Interfaces, 2021, 13, 54610-54619.	8.0	1
75	Observation of a molecular muonium polaron and its application to probing magnetic and electronic states. Physical Review B, 2021, 104, .	3.2	0
76	Unique properties of geoinspired nanotubes as water nanocontainer. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e436-e436.	0.1	0
77	Specific water structure in a geo-inspired nanotube and interrelated dynamics. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, C1009-C1009.	0.1	0