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	Nonadiabatic Dynamics of Polaron Hopping and Coupling with Water on Reduced TiO₂. Journal of Physical Chemistry Letters, 2022, 13, 857-863.	4.6	6
2	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
3	Structure and Oxygen Evolution Activity of Î²-NiOOH: Where Are the Protons?. ACS Catalysis, 2022, 12, 295-304.	11.2	28
4	Kinetic Monte Carlo modeling of oxide thin film growth. Journal of Chemical Physics, 2022, 156, .	3.0	3
5	The unique carrier mobility of Janus MoSSe/GaN heterostructures. Frontiers of Physics, 2021, 16, 1.	5.0	18
6	The unique carrier mobility of monolayer Janus MoSSe nanoribbons: a first-principles study. Dalton Transactions, 2021, 50, 10252-10260.	3.3	8
7	Enhanced Spinâ€“Orbit Coupling in Heavy Metals via Molecular Coupling. ACS Applied Materials & Interfaces, 2021, 13, 5228-5234.	8.0	10
8	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
9	Amorphous Domains in Black Titanium Dioxide. Advanced Materials, 2021, 33, e2100407.	21.0	36
10	Observation of a molecular muonium polaron and its application to probing magnetic and electronic states. Physical Review B, 2021, 104, .	3.2	0
11	Recent advances in low-dimensional Janus materials: theoretical and simulation perspectives. Materials Advances, 2021, 2, 7543-7558.	5.4	38
12	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
13	Subspace Occupancy-Constraining Potentials for Modeling Polaron Formation. Journal of Physical Chemistry C, 2021, 125, 26354-26362.	3.1	4
14	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
15	Termination Effects in Aluminosilicate and Aluminogermanate Imogolite Nanotubes: A Density Functional Theory Study. Crystals, 2020, 10, 1051.	2.2	6
16	The oxygen vacancy in Li-ion battery cathode materials. Nanoscale Horizons, 2020, 5, 1453-1466.	8.0	77
17	Activity and selectivity of CO₂ photoreduction on catalytic materials. Dalton Transactions, 2020, 49, 12918-12928.	3.3	13
18	Work Function Evolution in Li Anode Processing. Advanced Energy Materials, 2020, 10, 2000520.	19.5	40

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19	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
20	The <scp>ONETEP</scp> linear-scaling density functional theory program. Journal of Chemical Physics, 2020, 152, 174111.	3.0	94
21	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
22	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
23	Solid wetting-layers in inorganic nano-reactors: the water in imogolite nanotube case. Nanoscale Advances, 2020, 2, 1869-1877.	4.6	17
24	<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
25	Reversible spin storage in metal oxideâ€"fullerene heterojunctions. Science Advances, 2020, 6, eaax1085.	10.3	10
26	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
27	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
28	Unique properties of geoinspired nanotubes as water nanocontainer. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e436-e436.	0.1	0
29	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
30	Structural resolution of inorganic nanotubes with complex stoichiometry. Nature Communications, 2018, 9, 2033.	12.8	33
31	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
32	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
33	Chemically Selective Alternatives to Photoferroelectrics for Polarizationâ€Enhanced Photocatalysis: The Untapped Potential of Hybrid Inorganic Nanotubes. Advanced Science, 2017, 4, 1600153.	11.2	29
34	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
35	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
36	Optimization of constrained density functional theory. Physical Review B, 2016, 94, .	3.2	19

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37	Supercell convergence of charge-transfer energies in pentacene molecular crystals from constrained DFT. Physical Review B, 2016, 93, .	3.2	18
38	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
39	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
40	Beating the Stoner criterion using molecular interfaces. Nature, 2015, 524, 69-73.	27.8	151
41	What is the orientation of the tip in a scanning tunneling microscope?. Progress in Surface Science, 2015, 90, 223-238.	8.3	18
42	(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
43	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
44	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
45	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:mo>/ Physical Review B, 2014, 90, .	3.2	50
46	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
47	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
48	Polymorphism and isomerisation of an azobenzene derivative on gold. Chemical Communications, 2011, 47, 8662.	4.1	3
49	The effect of temperature on the internal dynamics of dansylated POPAM dendrimers. RSC Advances, 2011, 1, 1778.	3.6	9
50	Chemical Resolution at Ionic Crystal Surfaces Using Dynamic Atomic Force Microscopy with Metallic Tips. Physical Review Letters, 2011, 106, 216102.	7.8	56
51	The effect of van der Waals interactions on the properties of intrinsic defects in graphite. Carbon, 2010, 48, 4145-4161.	10.3	37
52	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
53	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
54	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

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55	Hydroxyl vacancies in single-walled aluminosilicate and aluminogermanate nanotubes. Journal of Physics Condensed Matter, 2009, 21, 195301.	1.8	20
56	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
57	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
58	Creating pseudo-Kondo resonances by field-induced diffusion of atomic hydrogen. Nanotechnology, 2008, 19, 305701.	2.6	16
59	Geometric Structure ofTiO2(011)(2Ã—1). Physical Review Letters, 2008, 101, 185501.	7.8	87
60	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
61	Detection of spin-states in Mn-doped gallium arsenide films. Nanotechnology, 2007, 18, 044006.	2.6	1
62	Including the probe tip in theoretical models of inelastic scanning tunneling spectroscopy: CO on Cu(100). Physical Review B, 2007, 76, .	3.2	27
63	Extremely Strong and Readily Accessible AAAâ˜DDD Triple Hydrogen Bond Complexes. Journal of the American Chemical Society, 2007, 129, 476-477.	13.7	103
64	Adsorption of Organic Molecules on Gold Electrodes. Journal of Physical Chemistry C, 2007, 111, 13879-13885.	3.1	22
65	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
66	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
67	C₆₀ on Gold: Adsorption, Motion, and Viscosity. Small, 2007, 3, 1694-1698.	10.0	19
68	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
69	Macroscopic transport by synthetic molecular machines. Nature Materials, 2005, 4, 704-710.	27.5	685
70	Understanding the Cosolvation Effect of Dendrimers. Journal of Chemical Theory and Computation, 2005, 1, 194-200.	5.3	4
71	Modelling of the Adsorption of C60 on the Au(110) Surface. ChemPhysChem, 2004, 5, 245-248.	2.1	33
72	A Generic Basis for Some Simple Light-Operated Mechanical Molecular Machines. Journal of the American Chemical Society, 2004, 126, 12210-12211.	13.7	199

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73	Modeling the Adsorption of Alkanes on an Au(111) Surface. Langmuir, 2003, 19, 7335-7340.	3.5	57
74	Molecular Dynamics of a Dendrimerâ"Dye Guestâ"Host System. Journal of the American Chemical Society, 2003, 125, 7388-7393.	13.7	53
75	Kinetics of Place-Exchange Reactions of Thiols on Gold Nanoparticles. Langmuir, 2003, 19, 5172-5174.	3.5	119
76	Theory of Scanning Tunneling Microscopy and Applications in Catalysis. , 0, , 97-118.		1
77	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