Stefano Fabris

List of Publications by Year
in descending order

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81	26,261	76326 40	56724 83
papers	citations	h-index	g-index

83	83	83	29541
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
2	Electron Localization Determines Defect Formation on Ceria Substrates. Science, 2005, 309, 752-755.	12.6	1,211
3	Counting electrons on supported nanoparticles. Nature Materials, 2016, 15, 284-288.	27.5	469
4	Dual Path Mechanism in the Thermal Reduction of Graphene Oxide. Journal of the American Chemical Society, 2011, 133, 17315-17321.	13.7	426
5	Creating single-atom Pt-ceria catalysts by surface step decoration. Nature Communications, 2016, 7, 10801.	12.8	388
6	Taming multiple valency with density functionals:â€ƒA case study of defective ceria. Physical Review B, 2005, 71, .	3.2	383
7	Structure of the catalytically active copperâ€“ceria interfacial perimeter. Nature Catalysis, 2019, 2, 334-341.	34.4	368
8	Electronic and Atomistic Structures of Clean and Reduced Ceria Surfaces. Journal of Physical Chemistry B, 2005, 109, 22860-22867.	2.6	358
9	A stabilization mechanism of zirconia based on oxygen vacancies only. Acta Materialia, 2002, 50, 5171-5178.	7.9	330
10	Reaction Mechanisms for the CO Oxidation on Au/CeO₂ Catalysts: Activity of Substitutional Au³⁺/Au⁺ Cations and Deactivation of Supported Au⁺ Adatoms. Journal of the American Chemical Society, 2009, 131, 10473-10483.	13.7	304
11	CO Adsorption and Oxidation on Ceria Surfaces from DFT+U Calculations. Journal of Physical Chemistry C, 2008, 112, 8643-8648.	3.1	264
12	Nanofaceted Pdï£¿O Sites in Pdï£¿Ce Surface Superstructures: Enhanced Activity in Catalytic Combustion of Methane. Angewandte Chemie - International Edition, 2009, 48, 8481-8484.	13.8	256
13	Initial Stages of Oxidation on Graphitic Surfaces: Photoemission Study and Density Functional Theory Calculations. Journal of Physical Chemistry C, 2009, 113, 9009-9013.	3.1	224
14	Electronic Structure of Surface-supported Bis(phthalocyaninato) terbium(III) Single Molecular Magnets. Nano Letters, 2008, 8, 3364-3368.	9.1	183
15	Reply to â€œComment on â€˜Taming multiple valency with density functionals: A case study of defective ceria' â€• Physical Review B, 2005, 72, .	3.2	177
16	Mechanisms for Oxidative Unzipping and Cutting of Graphene. Nano Letters, 2012, 12, 17-21.	9.1	129
17	Templated Growth of Metal-Organic Coordination Chains at Surfaces. Angewandte Chemie - International Edition, 2005, 44, 6142-6145.	13.8	125
18	Hydrogen and Coordination Bonding Supramolecular Structures of Trimesic Acid on Cu(110). Journal of Physical Chemistry A, 2007, 111, 12589-12603.	2.5	118

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19	Role of surface peroxo and superoxo species in the low-temperature oxygen buffering of ceria: Density functional theory calculations. Physical Review B, 2007, 75, .	3.2	112
20	Surface Precursors and Reaction Mechanisms for the Thermal Reduction of Graphene Basal Surfaces Oxidized by Atomic Oxygen. Journal of Physical Chemistry C, 2011, 115, 4730-4737.	3.1	101
21	Interaction of Hydrogen with Cerium Oxide Surfaces:â€‰a Quantum Mechanical Computational Study. Journal of Physical Chemistry B, 2006, 110, 19380-19385.	2.6	85
22	Oxide-based nanomaterials for fuel cell catalysis: the interplay between supported single Pt atoms and particles. Catalysis Science and Technology, 2017, 7, 4315-4345.	4.1	84
23	Thermodynamic, electronic and structural properties of Cu/CeO $_2$2 surfaces and interfaces from first-principles DFT+U calculations. Journal of Chemical Physics, 2010, 133, 234705.	3.0	83
24	Relative energetics and structural properties of zirconia using a self-consistent tight-binding model. Physical Review B, 2000, 61, 6617-6630.	3.2	82
25	Catalytic Proton Dynamics at the Water/Solid Interface of Ceria-Supported Pt Clusters. Journal of the American Chemical Society, 2016, 138, 11560-11567.	13.7	82
26	Water oxidation surface mechanisms replicated by a totally inorganic tetraruthenium–oxo molecular complex. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 4917-4922.	7.1	80
27	Fluxionality of Au Clusters at Ceria Surfaces during CO Oxidation: Relationships among Reactivity, Size, Cohesion, and Surface Defects from DFT Simulations. Journal of Physical Chemistry Letters, 2013, 4, 2256-2263.	4.6	76
28	Monitoring Two-Dimensional Coordination Reactions:Â Directed Assembly of Coâ^'Terephthalate Nanosystems on Au(111). Journal of Physical Chemistry B, 2006, 110, 5627-5632.	2.6	74
29	Spin and orbital configuration of metal phthalocyanine chains assembled on the Au(110) surface. Physical Review B, 2013, 87, .	3.2	67
30	Oxygen Dissociation by Concerted Action of Di-Iron Centers in Metal–Organic Coordination Networks at Surfaces: Modeling Non-Heme Iron Enzymes. Nano Letters, 2011, 11, 5414-5420.	9.1	66
31	Free energy and molecular dynamics calculations for the cubic-tetragonal phase transition in zirconia. Physical Review B, 2001, 63, .	3.2	64
32	Atomistic Structure of Cobalt-Phosphate Nanoparticles for Catalytic Water Oxidation. ACS Nano, 2012, 6, 10497-10504.	14.6	62
33	Reactivity of atomically dispersed Pt²⁺ species towards H₂: model Pt–CeO₂ fuel cell catalyst. Physical Chemistry Chemical Physics, 2016, 18, 7672-7679.	2.8	61
34	Σ13(101Â¯4)twin inα–Al2O3:A model for a general grain boundary. Physical Review B, 2001, 64, .	3.2	59
35	Enhanced Oxygen Buffering by Substitutional and Interstitial Ni Point Defects in Ceria: A First-Principles DFT+U Study. Journal of Physical Chemistry C, 2010, 114, 10221-10228.	3.1	52
36	Bulk Hydroxylation and Effective Water Splitting by Highly Reduced Cerium Oxide: The Role of O Vacancy Coordination. ACS Catalysis, 2018, 8, 4354-4363.	11.2	52

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37	Effects of Thermal Fluctuations on the Hydroxylation and Reduction of Ceria Surfaces by Molecular H₂. Journal of Physical Chemistry C, 2015, 119, 21567-21573.	3.1	50
38	First-principles analysis of cation segregation at grain boundaries in Î±-Al2O3. Acta Materialia, 2003, 51, 71-86.	7.9	49
39	Role of Cluster Morphology in the Dynamics and Reactivity of Subnanometer Pt Clusters Supported on Ceria Surfaces. Journal of Physical Chemistry C, 2014, 118, 21014-21020.	3.1	47
40	Energetics of Water Oxidation Catalyzed by Cobalt Oxide Nanoparticles: Assessing the Accuracy of DFT and DFT+U Approaches against Coupled Cluster Methods. Journal of Physical Chemistry Letters, 2013, 4, 4223-4230.	4.6	42
41	Distinct Physicochemical Properties of the First Ceria Monolayer on Cu(111). Journal of Physical Chemistry C, 2012, 116, 6677-6684.	3.1	40
42	Reaction Mechanisms of Water Splitting and H₂ Evolution by a Ru(II)-Pincer Complex Identified with Ab Initio Metadynamics Simulations. ACS Catalysis, 2012, 2, 1500-1506.	11.2	39
43	Quantitative Analysis of the Oxidation State of Cobalt Oxides by Resonant Photoemission Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 6129-6136.	4.6	39
44	Molecule-Driven Substrate Reconstruction in the Two-Dimensional Self-Organization of Fe-Phthalocyanines on Au(110). Journal of Physical Chemistry C, 2012, 116, 6251-6258.	3.1	38
45	Copper-ceria interaction: A combined photoemission and DFT study. Applied Surface Science, 2013, 267, 12-16.	6.1	37
46	Varying molecular interactions by coverage in supramolecular surface chemistry. Chemical Communications, 2012, 48, 534-536.	4.1	34
47	PrismaticÎ£3(101Â¯0)twin boundary inÎ±â^'Al2O3investigated by density functional theory and transmission electron microscopy. Physical Review B, 2002, 66, .	3.2	31
48	Defect-Controlled Transport Properties of Metallic Atoms along Carbon Nanotube Surfaces. Physical Review Letters, 2007, 99, 046803.	7.8	31
49	A first principles study of water oxidation catalyzed by a tetraruthenium-oxo core embedded in polyoxometalate ligands. Physical Chemistry Chemical Physics, 2011, 13, 7666.	2.8	31
50	Adsorption of alkali adatoms on graphene supported by the Au/Ni(111) surface. Physical Review B, 2015, 92, .	3.2	30
51	Properties of Pt-supported Co nanomagnets from relativistic density functional theory calculations. Physical Review B, 2008, 78, .	3.2	26
52	Tertiary Chiral Domains Assembled by Achiral Metalâ^'Organic Complexes on Cu(110). Journal of Physical Chemistry C, 2010, 114, 13020-13025.	3.1	26
53	Structural Phases of Ordered FePc-Nanochains Self-Assembled on Au(110). Langmuir, 2012, 28, 13232-13240.	3.5	26
54	Importance of semicore states in GW calculations for simulating accurately the photoemission spectra of metal phthalocyanine molecules. Journal of Chemical Physics, 2012, 136, 174310.	3.0	23

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55	Probing the Reactivity of Pt/Ceria Nanocatalysts toward Methanol Oxidation: From Ionic Single-Atom Sites to Metallic Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 17917-17927.	3.1	22
56	Experimental and Theoretical Study on the Electronic Interaction between Rh Adatoms and CeOx Substrate in Dependence on a Degree of Cerium Oxide Reduction. Journal of Physical Chemistry C, 2016, 120, 5468-5476.	3.1	21
57	Ultimate dispersion of metallic and ionic platinum on ceria. Journal of Materials Chemistry A, 2019, 7, 13019-13028.	10.3	21
58	Formation of Hybrid Electronic States in FePc Chains Mediated by the Au(110) Surface. Journal of Physical Chemistry C, 2012, 116, 8657-8663.	3.1	20
59	Programming Hierarchical Supramolecular Nanostructures by Molecular Design. Journal of Physical Chemistry C, 2013, 117, 3440-3445.	3.1	20
60	Unveiling Oxygen Vacancy Superstructures in Reduced Anatase Thin Films. Nano Letters, 2020, 20, 6444-6451.	9.1	20
61	CuFeO₂â€“Water Interface under Illumination: Structural, Electronic, and Catalytic Implications for the Hydrogen Evolution Reaction. ACS Catalysis, 2021, 11, 1897-1910.	11.2	20
62	Structure and Moleculeâ€“Substrate Interaction in a Co-octaethyl Porphyrin Monolayer on the Ag(110) Surface. Journal of Physical Chemistry C, 2011, 115, 11560-11568.	3.1	19
63	Adatom and Nanoparticle Dynamics on Single-Atom Catalyst Substrates. ACS Catalysis, 2022, 12, 4859-4871.	11.2	19
64	Thermodynamic Stability and Native Point Defects of CuFeO₂ Photocathodes in Dry and Electrochemical Environments. Journal of Physical Chemistry C, 2019, 123, 29589-29598.	3.1	17
65	Water Adsorption and Dissociation at Metal-Supported Ceria Thin Films: Thickness and Interface-Proximity Effects Studied with DFT+U Calculations. Journal of Physical Chemistry C, 2015, 119, 2537-2544.	3.1	16
66	Nanometer-Range Strain Distribution in Layered Incommensurate Systems. Physical Review Letters, 2012, 109, 266102.	7.8	15
67	Effects of Thermal Electronic Excitations on the Diffusion of Oxygen Adatoms on Graphene. Journal of Physical Chemistry A, 2016, 120, 2607-2613.	2.5	11
68	Heterogeneous reactions of SO2 on the hematite(0001) surface. Journal of Chemical Physics, 2018, 149, 194703.	3.0	10
69	Dynamical Solvent Effects on the Charge and Reactivity of Ceria-Supported Pt Nanoclusters. Journal of Physical Chemistry C, 2018, 122, 27507-27515.	3.1	10
70	Three-Dimensional Tomography of the Beryllium Fermi Surface: Surface Charge Redistribution. Physical Review Letters, 2007, 99, 166403.	7.8	9
71	Water Oxidation by Ru-Polyoxometalate Catalysts: Overpotential Dependency on the Number and Charge of the Metal Centers. Inorganics, 2015, 3, 374-387.	2.7	8
72	Establishing best practices to model the electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CuFeO</mml:mi><mml:mn>2</mml:mn></mml:msub></r from first principles. Physical Review B, 2020, 101, .	3.2	8

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73	Oxygen Evolution Reaction on the Fe₃O₄(001) Surface: Theoretical Insights into the Role of Terminal and Bridging Oxygen Atoms. Journal of Physical Chemistry C, 2021, 125, 18752-18761.	3.1	8
74	Two different mechanisms of stabilization of regular Ï€-stacks of radicals in switchable dithiazolyl-based materials. Journal of Materials Chemistry C, 2020, 8, 5437-5448.	5.5	7
75	QMMMW: A wrapper for QM/MM simulations with Quantum ESPRESSO Âand LAMMPS. Computer Physics Communications, 2015, 195, 191-198.	7.5	6
76	Self-texturizing electronic properties of a 2-dimensional GdAu₂ layer on Au(111): the role of out-of-plane atomic displacement. Nanoscale, 2017, 9, 17342-17348.	5.6	6
77	Metallization of the C60/Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2010, 132, 234710.	3.0	5
78	Oxidation of Gas-Phase and Supported Pt Nanoclusters: An Ab Initio Investigation. Journal of Physical Chemistry C, 2022, 126, 10880-10888.	3.1	4
79	Interface structure and reactivity of water-oxidation Ruâ€“polyoxometalate catalysts on functionalized graphene electrodes. Physical Chemistry Chemical Physics, 2014, 16, 5333-5341.	2.8	3
80	Can Atomic Buckling Control a Chemical Reaction? The Case of Dehydrogenation of Phthalocyanine Molecules on GdAu₂/Au(111). Journal of Physical Chemistry C, 2019, 123, 6496-6501.	3.1	3
81	Ab-Initio Theory of Grain-Boundary Segregation in Î±-Alumina: Energetics, Atomistic and Electronic Structures. Materials Research Society Symposia Proceedings, 2002, 751, 1.	0.1	1