Sergio Tosoni

List of Publications by Citations

93 papers	2,635 citations	27 h-index	48 g-index
100 ext. papers	3,158 ext. citations	6.3 avg, IF	5.77 L-index

#	Paper	IF	Citations
93	Increasing Oxide Reducibility: The Role of Metal/Oxide Interfaces in the Formation of Oxygen Vacancies. *ACS Catalysis*, **2017**, 7, 6493-6513	13.1	375
92	Vibrational spectrum of brucite, Mg(OH)2: a periodic ab initio quantum mechanical calculation including OH anharmonicity. *Chemical Physics Letters*, **2004**, 396, 308-315	2.5	122
91	Accurate quantum chemical energies for the interaction of hydrocarbons with oxide surfaces: CH(4)/MgO(001). *Physical Chemistry Chemical Physics*, **2010**, 12, 14330-40	3.6	113
90	Quantum mechanical calculation of the OH vibrational frequency in crystalline solids. *Molecular Physics*, **2005**, 103, 2549-2558	1.7	89
89	Hydrogen Adsorption, Dissociation, and Spillover on Ru10 Clusters Supported on Anatase TiO2 and Tetragonal ZrO2 (101) Surfaces. *ACS Catalysis*, **2015**, 5, 5486-5495	13.1	85
88	Interaction of glycine with isolated hydroxyl groups at the silica surface: first principles B3LYP periodic simulation. *Langmuir*, **2006**, 22, 6593-604	4	77
87	Water adsorption on the stoichiometric (001) and (010) surfaces of hydroxyapatite: a periodic B3LYP study. *Langmuir*, **2009**, 25, 2188-98	4	73
86	Role of dispersive interactions in layered materials: a periodic B3LYP and B3LYP-D* study of Mg(OH)2, Ca(OH)2 and kaolinite. *Journal of Materials Chemistry*, **2009**, 19, 2564		70
85	Does silica surface catalyse peptide bond formation? New insights from first-principles calculations. *ChemPhysChem*, **2006**, 7, 157-63	3.2	70
84	Theoretical approaches to excited-state-related phenomena in oxide surfaces. *Chemical Reviews*, **2013**, 113, 4456-95	68.1	69
83	Infrared Spectra of Hydrogen-Bonded Ionic Crystals:Ab Initio Study of Mg(OH)2and Be(OH)2. *Journal of Physical Chemistry B*, **2004**, 108, 13632-13637	3.4	63
82	Electronic Structure of F-Doped Bulk Rutile, Anatase, and Brookite Polymorphs of TiO2. *Journal of Physical Chemistry C*, **2012**, 116, 12738-12746	3.8	62
81	Hydrogen Bond in Layered Materials: Structural and Vibrational Properties of Kaolinite by a Periodic B3LYP Approach. *Chemistry of Materials*, **2006**, 18, 2135-2143	9.6	61
80	Adsorption of Ruthenium Atoms and Clusters on Anatase TiO2 and Tetragonal ZrO2(101) Surfaces: A Comparative DFT Study. *Journal of Physical Chemistry C*, **2015**, 119, 10856-10868	3.8	59
79	A comparison between plane wave and Gaussian-type orbital basis sets for hydrogen bonded systems: formic acid as a test case. *Journal of Chemical Physics*, **2007**, 127, 154102	3.9	59
78	A DFT study of the acidBase properties of anatase TiO2 and tetragonal ZrO2 by adsorption of CO and CO2 probe molecules. *Surface Science*, **2016**, 652, 163-171	1.8	54
77	Effect of Alkali Metals Interstitial Doping on Structural and Electronic Properties of WO3. *Journal of Physical Chemistry C*, **2014**, 118, 3000-3006	3.8	54

76	Acid-base interactions and secondary structures of poly-L-lysine probed by 15N and 13C solid state NMR and Ab initio model calculations. *Journal of Physical Chemistry B*, **2008**, 112, 15604-15	3.4	49
75	Al- and Ga-Doped TiO2, ZrO2, and HfO2: The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. *Chemistry of Materials*, **2015**, 27, 3936-3945	9.6	39
74	Acetic acid ketonization on tetragonal zirconia: Role of surface reduction. *Journal of Catalysis*, **2016** , 344, 465-473	7.3	35
73	Role of Heterojunction in Charge Carrier Separation in Coexposed Anatase (001)-(101) Surfaces. *Journal of Physical Chemistry Letters*, **2019**, 10, 2372-2377	6.4	33
72	Oxide-Supported Gold Clusters and Nanoparticles in Catalysis: A Computational Chemistry Perspective. *ChemCatChem*, **2019**, 11, 73-89	5.2	32
71	Comparison between Gaussian-type orbitals and plane wave ab initio density functional theory modeling of layer silicates: talc [Mg3Si4O10(OH)2] as model system. *Journal of Chemical Physics*, **2013**, 139, 204101	3.9	32
70	Peptide bond formation activated by the interplay of Lewis and Brønsted catalysts. *Chemical Physics Letters*, **2005**, 408, 295-301	2.5	30
69	Evidence of Charge Transfer to Atomic and Molecular Adsorbates on ZnO/X(111) (X = Cu, Ag, Au) Ultrathin Films. Relevance for Cu/ZnO Catalysts. *ACS Catalysis*, **2018**, 8, 4110-4119	13.1	29
68	Origin of Optical Excitations in Fluorine-Doped Titania from Response Function Theory: Relevance to Photocatalysis. *Journal of Physical Chemistry Letters*, **2012**, 3, 2269-74	6.4	28
67	DFT Study of CO2Activation on Doped and Ultrathin MgO Films.. *Journal of Physical Chemistry C*, **2015**, 119, 27594-27602	3.8	27
66	Relative Stability of F-Covered TiO2 Anatase (101) and (001) Surfaces from Periodic DFT Calculations and ab Initio Atomistic Thermodynamics. *Journal of Physical Chemistry C*, **2014**, 118, 13667-13673	3.8	27
65	CO Adsorption on Graphite-like ZnO Bilayers Supported on Cu(111), Ag(111), and Au(111) Surfaces. *Journal of Physical Chemistry C*, **2017**, 121, 27453-27461	3.8	27
64	The compressional behaviour and the mechanical properties of talc [Mg3Si4O10(OH)2]: a density functional theory investigation. *Physics and Chemistry of Minerals*, **2014**, 41, 639-650	1.6	26
63	How Growing Conditions and Interfacial Oxygen Affect the Final Morphology of MgO/Ag(100) Films. *Journal of Physical Chemistry C*, **2014**, 118, 26091-26102	3.8	26
62	Turning a Nonreducible into a Reducible Oxide via Nanostructuring: Opposite Behavior of Bulk ZrO2 and ZrO2 Nanoparticles Toward H2 Adsorption. *Journal of Physical Chemistry C*, **2016**, 120, 15329-15337	3.8	26
61	Band Gap of 3D Metal Oxides and Quasi-2D Materials from Hybrid Density Functional Theory: Are Dielectric-Dependent Functionals Superior?. *Journal of Chemical Theory and Computation*, **2019**, 15, 6294-6312	5.4	25
60	Nature of Sintering-Resistant, Single-Atom Ru Species Dispersed on Zirconia-Based Catalysts: A DFT and FTIR Study of CO Adsorption. *ChemCatChem*, **2018**, 10, 2634-2645	5.2	24
59	Quantum confinement in group III-V semiconductor 2D nanostructures. *Nanoscale*, **2020**, 12, 17494-17501	7.7	24

58	Nitrogen doping in coexposed (001)-(101) anatase TiO surfaces: a DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 21497-21505	3.6	23
57	Bandgap engineering through nanoporosity. *Nanoscale*, **2014**, 6, 1181-7	7.7	23
56	Theoretical study of the Fluorine doped anatase surfaces. *Surface Science*, **2013**, 618, 154-158	1.8	23
55	Trends in Adhesion Energies of Gold on MgO(100), Rutile TiO2(110), and CeO2(111) Surfaces: A Comparative DFT Study. *Journal of Physical Chemistry C*, **2017**, 121, 28328-28338	3.8	23
54	Hydrophobic Behavior of Dehydroxylated Silica Surfaces: A B3LYP Periodic Study. *Journal of Physical Chemistry C*, **2010**, 114, 19984-19992	3.8	22
53	A DFT study of Ni clusters deposition on titania and zirconia (101) surfaces. *Surface Science*, **2016**, 646, 230-238	1.8	20
52	Structural and electronic properties of bulk and ultrathin layers of V2O5 and MoO3. *Computational Materials Science*, **2019**, 163, 230-240	3.2	20
51	A DFT Study of the Reactivity of Anatase TiO2 and Tetragonal ZrO2 Stepped Surfaces Compared to the Regular (101) Terraces. *ChemPhysChem*, **2015**, 16, 3642-51	3.2	19
50	Nature of SrTiO/TiO (anatase) heterostructure from hybrid density functional theory calculations. *Journal of Chemical Physics*, **2020**, 152, 184704	3.9	18
49	Charge Carriers Cascade in a Ternary TiO2/TiO2/ZnS Heterojunction: A DFT Study. *ChemCatChem*, **2020**, 12, 2097-2105	5.2	16
48	Stabilizing gold adatoms by thiophenyl derivatives: a possible route toward metal redispersion. *Journal of the American Chemical Society*, **2012**, 134, 11161-7	16.4	16
47	Zeolitic-type Brønsted-Lowry sites distribution imaged on clinochlore. *American Mineralogist*, **2011**, 96, 1461-1466	2.9	15
46	Enhanced Functional Properties of Ti3C2Tx MXenes as Negative Electrodes in Sodium-Ion Batteries by Chemical Tuning. *Small Methods*, **2020**, 4, 2000314	12.8	14
45	Theoretical treatment of semiconductor heterojunctions for photocatalysis: the WO/BiVO interface. *Journal of Physics Condensed Matter*, **2019**, 31, 434001	1.8	14
44	Band Gap in Magnetic Insulators from a Charge Transition Level Approach. *Journal of Chemical Theory and Computation*, **2020**, 16, 3786-3798	6.4	13
43	Dopant-Induced Diffusion Processes at Metal□Oxide Interfaces Studied for Iron- and Chromium-Doped MgO/Mo(001) Model Systems. *Journal of Physical Chemistry C*, **2016**, 120, 13604-13609	3.8	13
42	Theoretical Study of Atomic Fluorine Diffusion through Bulk TiO2 Polymorphs. *Journal of Physical Chemistry C*, **2013**, 117, 5855-5860	3.8	13
41	Influence of surface hydroxylation on the Ru atom diffusion on the ZrO2(101) surface: A DFT study. *Surface Science*, **2017**, 664, 87-94	1.8	12

40	TiO and ZrO in biomass conversion: why catalyst reduction helps. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2018**, 376,	3	12
39	Interaction Between Gold Atoms and Thio-Aryl Ligands on the Au(111) Surface. *Journal of Physical Chemistry C*, **2011**, 115, 24871-24879	3.8	11
38	Role of surface termination in forming type-II photocatalyst heterojunctions: the case of TiO/BiVO. *Journal of Physics Condensed Matter*, **2021**, 33, 075001	1.8	11
37	Determination of Silica and Germania Film Network Structures on Ru(0001) at the Atomic Scale. *Journal of Physical Chemistry C*, **2019**, 123, 7889-7897	3.8	11
36	Rational Design of Semiconductor Heterojunctions for Photocatalysis. *Chemistry - A European Journal*, **2021**, 27, 13306-13317	4.8	11
35	Formation of Reversible Adducts by Adsorption of Oxygen on Ce□rO2: An Unusual □ Ionic Superoxide. *Journal of Physical Chemistry C*, **2019**, 123, 27088-27096	3.8	10
34	Phonon-mediated electron transport through CaO thin films. *Physical Review Letters*, **2015**, 114, 016804	7.4	10
33	Hydroxylated crystalline edingtonite silica faces as models for the amorphous silica surface. *Journal of Physics: Conference Series*, **2008**, 117, 012026	0.3	10
32	Spontaneous Oxidation of Ni Nanoclusters on MgO Monolayers Induced by Segregation of Interfacial Oxygen. *Journal of Physical Chemistry Letters*, **2015**, 6, 3104-9	6.4	9
31	Two-dimensional TiO x nanostructures on Au(111): a scanning tunneling microscopy and spectroscopy investigation. *2D Materials*, **2015**, 2, 045011	5.9	9
30	Nature and Role of Surface Junctions in BiOIO3 Photocatalysts. *Advanced Functional Materials*, **2021**, 31, 2009472	15.6	9
29	From Crystalline to Amorphous Germania Bilayer Films at the Atomic Scale: Preparation and Characterization. *Angewandte Chemie - International Edition*, **2019**, 58, 10903-10908	16.4	8
28	The epitaxial growth of ZnO films on Cu(111) surface: Thickness dependence. *Applied Surface Science*, **2019**, 483, 133-139	6.7	8
27	Nature of Point Defects in Single-Layer MoS2 Supported on Au(111). *Journal of Physical Chemistry C* , **2020**, 124, 12424-12431	3.8	8
26	Hydrogen Adsorption on Free-Standing and Ag□t Supported TiO2 Thin Films. *Journal of Physical Chemistry C*, **2019**, 123, 7952-7960	3.8	8
25	Azide-Alkyne Click Chemistry over a Heterogeneous Copper-Based Single-Atom Catalyst. *ACS Catalysis*, **2022**, 12, 2947-2958	13.1	8
24	Growth and Atomic-Scale Characterization of Ultrathin Silica and Germania Films: The Crucial Role of the Metal Support. *Chemistry - A European Journal*, **2021**, 27, 1870-1885	4.8	7
23	Prediction of optical properties of F centers in oxides from quasiparticle excitations. *Physical Review B*, **2012**, 85,	3.3	5

22	Structure of a Silica Thin Film on Oxidized Cu(111): Conservation of the Honeycomb Lattice and Role of the Interlayer. *Journal of Physical Chemistry C*, **2020**, 124, 20942-20949	3.8	5
21	Bonding Properties of Isolated Metal Atoms on Two-Dimensional Oxides. *Journal of Physical Chemistry C*, **2020**, 124, 20960-20973	3.8	5
20	Layered oxides as cathode materials for beyond-Li batteries: A computational study of Ca and Al intercalation in bulk V2O5 and MoO3. *Computational Materials Science*, **2021**, 191, 110324	3.2	5
19	Z-Scheme versus type-II junction in g-C3N4/TiO2 and g-C3N4/SrTiO3/TiO2 heterostructures. *Catalysis Science and Technology*, **2021**, 11, 3589-3598	5.5	5
18	Interface Oxygen Induced Internal Structures of Ultrathin MgO Islands Grown on Ag(100). *Journal of Physical Chemistry C*, **2020**, 124, 8834-8842	3.8	4
17	Structure and Band Alignment of InP Photocatalysts Passivated by TiO2 Thin Films. *Journal of Physical Chemistry C*, **2021**, 125, 11620-11627	3.8	4
16	CH3Br adsorption on MgO/Mo ultrathin films: A DFT study. *Surface Science*, **2018**, 672-673, 1-6	1.8	3
15	Cluster Catalysis with Lattice Oxygen: Tracing Oxygen Transport from a Magnetite (001) Support onto Small Pt Clusters. *ACS Catalysis*, **2021**, 11, 9519-9529	13.1	3
14	Continuous network structure of two-dimensional silica across a supporting metal step edge: An atomic scale study. *Physical Review Materials*, **2021**, 5,	3.2	3
13	Structure and dynamics of CaO films: A computational study of an effect of external static electric field. *Physical Review B*, **2017**, 95,	3.3	2
12	Role of support in tuning the properties of single atom catalysts: Cu, Ag, Au, Ni, Pd, and Pt adsorption on SiO/Ru, SiO/Pt, and SiO/Si ultrathin films. *Journal of Chemical Physics*, **2021**, 154, 134706	3.9	2
11	Assessing the film-substrate interaction in germania films on reconstructed Au(111). *Physical Review B*, **2019**, 100,	3.3	2
10	WO/BiVO Photoanodes: Facets Matching at the Heterojunction and BiVO Layer Thickness Effects. *ACS Applied Energy Materials*, **2021**, 4, 8421-8431	6.1	2
9	From Crystalline to Amorphous Germania Bilayer Films at the Atomic Scale: Preparation and Characterization. *Angewandte Chemie*, **2019**, 131, 11019-11024	3.6	1
8	Infrared Spectra of Hydrogen-Bonded Ionic Crystals: Ab initio Study of Mg(OH)2 and Be(OH)2.. *ChemInform*, **2004**, 35, no		1
7	Vibrational Properties of CO Adsorbed on Au Single Atom Catalysts on TiO2(101), ZrO2(101), CeO2(111), and LaFeO3(001) Surfaces: A DFT Study. *Topics in Catalysis*,1	2.3	1
6	Growth and characterization of Ca-Mo mixed oxide films on Mo(001). *Journal of Chemical Physics*, **2019**, 151, 234708	3.9	1
5	Precursor chemistry of h-BN: adsorption, desorption, and decomposition of borazine on Pt(110). *Physical Chemistry Chemical Physics*, **2020**, 22, 11704-11712	3.6	0

4	Interface-Driven Assembly of Pentacene/MoS Lateral Heterostructures.. *Journal of Physical Chemistry C*, **2022**, 126, 1132-1139	3.8	0
3	Structural and electronic properties of TiO2 from first principles calculations **2021**, 67-85		0
2	Computational study of group III-V semiconductors and their interaction with oxide thin films. *Solid-State Electronics*, **2021**, 184, 108038	1.7	0
1	Back Cover: Enhanced Functional Properties of Ti3C2Tx MXenes as Negative Electrodes in Sodium-Ion Batteries by Chemical Tuning (Small Methods 9/2020). *Small Methods*, **2020**, 4, 2070037	12.8	