Gianfranco Pacchioni

List of Publications by Year in Descending Order

596 papers	32,034 citations	90 h-index	151 g-index
638 ext. papers	34,201 ext. citations	5.1 avg, IF	7.61 L-index

#	Paper	IF	Citations
596	Density Functional Theory Estimate of Halide Perovskite Band Gap: When Spin Orbit Coupling Helps. *Journal of Physical Chemistry C*, **2022**, 126, 2184-2198	3.8	3
595	A DFT study of formic acid decomposition on the stoichiometric SnO2 surface as a function of iso-valent doping. *Surface Science*, **2022**, 718, 122009	1.8	2
594	DFT study of electronic properties of N-doped ZnO and ZnO/Cu(111) bilayer films. *Surface Science*, **2022**, 716, 121978	1.8	2
593	From Li clusters to nanocatalysis: A brief tour of 40 years of cluster chemistry. *Inorganica Chimica Acta*, **2022**, 530, 120680	2.7	
592	Azide-Alkyne Click Chemistry over a Heterogeneous Copper-Based Single-Atom Catalyst. *ACS Catalysis*, **2022**, 12, 2947-2958	13.1	8
591	First principles approach to solar energy conversion efficiency of semiconductor heterojunctions. *Solar Energy*, **2022**, 236, 445-454	6.8	0
590	Defect engineering of oxide surfaces: dream or reality?. *Journal of Physics Condensed Matter*, **2022**, 34,	1.8	1
589	Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts. *Journal of the American Chemical Society*, **2021**, 143, 20431-20441	16.4	9
588	Prediction of 2D ferromagnetism and monovalent europium ions in EuBr/graphene heterojunctions. *Physical Chemistry Chemical Physics*, **2021**, 23, 25500-25506	3.6	1
587	Steric and Orbital Effects Induced by Isovalent Dopants on the Surface Chemistry of ZrO2. *ACS Catalysis*, **2021**, 11, 554-567	13.1	9
586	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
585	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
584	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
583	Structure and Band Alignment of InP Photocatalysts Passivated by TiO2 Thin Films. *Journal of Physical Chemistry C*, **2021**, 125, 11620-11627	3.8	4
582	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
581	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
580	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

579	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
578	Role of surface termination and quantum size in □CsPbX (X = Cl, Br, I) 2D nanostructures for solar light harvesting. *Physical Chemistry Chemical Physics*, **2021**, 23, 3031-3040	3.6	7
577	Structural and electronic properties of TiO2 from first principles calculations **2021**, 67-85		0
576	Nature and Role of Surface Junctions in BiOIO3 Photocatalysts. *Advanced Functional Materials*, **2021**, 31, 2009472	15.6	9
575	Band offset in semiconductor heterojunctions. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	4
574	WO/BiVO Photoanodes: Facets Matching at the Heterojunction and BiVO Layer Thickness Effects. *ACS Applied Energy Materials*, **2021**, 4, 8421-8431	6.1	2
573	Size and Shape Dependence of the Electronic Structure of Gold Nanoclusters on TiO. *Journal of Physical Chemistry Letters*, **2021**, 12, 8363-8369	6.4	2
572	Rational Design of Semiconductor Heterojunctions for Photocatalysis. *Chemistry - A European Journal*, **2021**, 27, 13306-13317	4.8	11
571	Iso-valent doping of reducible oxides: a comparison of rutile (110) and anatase (101) TiOsurfaces. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	2
570	Chemical Reactivity of Supported ZnO Clusters: Undercoordinated Zinc and Oxygen Atoms as Active Sites. *ChemPhysChem*, **2020**, 21, 2553-2564	3.2	3
569	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
568	Nature of SrTiO/TiO (anatase) heterostructure from hybrid density functional theory calculations. *Journal of Chemical Physics*, **2020**, 152, 184704	3.9	18
567	Applied vs fundamental research in heterogeneous photocatalysis: problems and perspectives. An introduction to 'physical principles of photocatalysis'. *Journal of Physics Condensed Matter*, **2020**, 32, 360301	1.8	2
566	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
565	Band Gap in Magnetic Insulators from a Charge Transition Level Approach. *Journal of Chemical Theory and Computation*, **2020**, 16, 3786-3798	6.4	13
564	Reductant composition influences the coordination of atomically dispersed Rh on anatase TiO2. *Catalysis Science and Technology*, **2020**, 10, 1597-1601	5.5	17
563	On the Real Nature of Rh Single-Atom Catalysts Dispersed on the ZrO2 Surface. *ChemCatChem*, **2020**, 12, 2595-2604	5.2	9
562	Charge Carriers Cascade in a Ternary TiO2/TiO2/ZnS Heterojunction: A DFT Study. *ChemCatChem*, **2020**, 12, 2097-2105	5.2	16

561	Unraveling the atomic structure, ripening behavior, and electronic structure of supported Au clusters. *Science Advances*, **2020**, 6, eaay4289	14.3	15
560	Quantum confinement in group III-V semiconductor 2D nanostructures. *Nanoscale*, **2020**, 12, 17494-17501	7.7	24
559	Influence of Strain on Acid–Basic Properties of Oxide Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 19126-19135	3.8	3
558	Characterization of Acid and Basic Sites on Zirconia Surfaces and Nanoparticles by Adsorbed Probe Molecules: A Theoretical Study. *Topics in Catalysis*, **2020**, 63, 1717-1730	2.3	6
557	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
556	Bonding Properties of Isolated Metal Atoms on Two-Dimensional Oxides. *Journal of Physical Chemistry C*, **2020**, 124, 20960-20973	3.8	5
555	Structural, electronic and photochemical properties of cerium-doped zirconium titanate. *Catalysis Today*, **2020**, 340, 49-57	5.3	7
554	Formation of Reversible Adducts by Adsorption of Oxygen on Ce□rO2: An Unusual □2 Ionic Superoxide. *Journal of Physical Chemistry C*, **2019**, 123, 27088-27096	3.8	10
553	Nitrogen doping in coexposed (001)-(101) anatase TiO surfaces: a DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 21497-21505	3.6	23
552	Electronic structure of CuWO: dielectric-dependent, self-consistent hybrid functional study of a Mott-Hubbard type insulator. *Journal of Physics Condensed Matter*, **2019**, 31, 145503	1.8	5
551	Structural evolution of atomically dispersed Pt catalysts dictates reactivity. *Nature Materials*, **2019**, 18, 746-751	27	250
550	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
549	From Crystalline to Amorphous Germania Bilayer Films at the Atomic Scale: Preparation and Characterization. *Angewandte Chemie*, **2019**, 131, 11019-11024	3.6	1
548	H2 Adsorption on Wurtzite ZnO and on ZnO/M(111) (M=Cu, Ag and Au) Bilayer Films. *ChemNanoMat*, **2019**, 5, 932-939	3.5	4
547	The epitaxial growth of ZnO films on Cu(111) surface: Thickness dependence. *Applied Surface Science*, **2019**, 483, 133-139	6.7	8
546	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
545	Nature of Atomically Dispersed Ru on Anatase TiO2: Revisiting Old Data Based on DFT Calculations. *Journal of Physical Chemistry C*, **2019**, 123, 7271-7282	3.8	6
544	Structural and electronic properties of bulk and ultrathin layers of V2O5 and MoO3. *Computational Materials Science*, **2019**, 163, 230-240	3.2	20

543	Oxide-Supported Gold Clusters and Nanoparticles in Catalysis: A Computational Chemistry Perspective. *ChemCatChem*, **2019**, 11, 73-89	5.2	32
542	Spontaneous Formation of Gold Cluster Anions on ZnO/Cu(111) Bilayer Films. *Journal of Physical Chemistry C*, **2019**, 123, 7644-7653	3.8	10
541	DFT Study of 17O NMR Spectroscopy Applied to Zirconia Surfaces and Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 21629-21638	3.8	7
540	Solar-driven chemistry: towards new catalytic solutions for a sustainable world. *Rendiconti Lincei*, **2019**, 30, 443-452	1.7	13
539	Theoretical treatment of semiconductor heterojunctions for photocatalysis: the WO/BiVO interface. *Journal of Physics Condensed Matter*, **2019**, 31, 434001	1.8	14
538	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
537	Growth and characterization of Ca-Mo mixed oxide films on Mo(001). *Journal of Chemical Physics*, **2019**, 151, 234708	3.9	1
536	O NMR as a measure of basicity of alkaline-earth oxide surfaces: A theoretical study. *Journal of Chemical Physics*, **2019**, 151, 224705	3.9	6
535	Assessing the film-substrate interaction in germania films on reconstructed Au(111). *Physical Review B*, **2019**, 100,	3.3	2
534	Hydrogen Adsorption on Free-Standing and Ag-Pt Supported TiO2 Thin Films. *Journal of Physical Chemistry C*, **2019**, 123, 7952-7960	3.8	8
533	CO Oxidation Promoted by a Pt4/TiO2 Catalyst: Role of Lattice Oxygen at the Metal/Oxide Interface. *Catalysis Letters*, **2019**, 149, 390-398	2.8	6
532	Role of Nanostructuring on the Properties of Oxide Materials: The Case of Zirconia Nanoparticles. *European Journal of Inorganic Chemistry*, **2019**, 2019, 751-761	2.3	3
531	Role of Metal/Oxide Interfaces in Enhancing the Local Oxide Reducibility. *Topics in Catalysis*, **2019**, 62, 1192-1201	2.3	10
530	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
529	Electronic structure of Al, Ga, In and Cu doped ZnO/Cu(111) bilayer films. *Physical Chemistry Chemical Physics*, **2018**, 21, 369-377	3.6	20
528	Atomic structure of a metal-supported two-dimensional germania film. *Physical Review B*, **2018**, 97,	3.3	14
527	Reduced sintering of mass-selected Au clusters on SiO by alloying with Ti: an aberration-corrected STEM and computational study. *Nanoscale*, **2018**, 10, 2363-2370	7.7	12
526	Controlling the charge state of supported nanoparticles in catalysis: lessons from model systems. *Chemical Society Reviews*, **2018**, 47, 8474-8502	58.5	93

525	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
524	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
523	Ultrathin silica films on Pd(111): Structure and adsorption properties. *Surface Science*, **2018**, 678, 118-123	1.8	19
522	CH3Br adsorption on MgO/Mo ultrathin films: A DFT study. *Surface Science*, **2018**, 672-673, 1-6	1.8	3
521	Support effects and reaction mechanism of acetylene trimerization over silica-supported Cu4 clusters: A DFT study. *Surface Science*, **2018**, 668, 125-133	1.8	8
520	Origin of Visible Light Photoactivity of the CeO2/ZnO Heterojunction. *ACS Applied Energy Materials*, **2018**, 1, 4247-4260	6.1	45
519	Oxygen Vacancy in Wurtzite ZnO and Metal-Supported ZnO/M(111) Bilayer Films (M = Cu, Ag and Au). *Journal of Physical Chemistry C*, **2018**, 122, 20880-20887	3.8	10
518	The Overproduction of Truth **2018**,		6
517	TiO and ZrO in biomass conversion: why catalyst reduction helps. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2018**, 376,	3	12
516	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. *Journal of Physics Condensed Matter*, **2018**, 30, 044003	1.8	47
515	Nature of stable single atom Pt catalysts dispersed on anatase TiO2. *Journal of Catalysis*, **2018**, 367, 104-114	7.3	117
514	Theory of Ferromagnetism in Reduced ZrO Nanoparticles. *ACS Omega*, **2018**, 3, 5301-5307	3.9	22
513	Bending Rigidity of 2D Silica. *Physical Review Letters*, **2018**, 120, 226101	7.4	11
512	CO Oxidation on a Au/TiO2 Nanoparticle Catalyst via the Au-Assisted Mars□an Krevelen Mechanism. *ACS Catalysis*, **2018**, 8, 6513-6525	13.1	71
511	ZrO2 Nanoparticles: a density functional theory study of structure, properties and reactivity. *Rendiconti Lincei*, **2017**, 28, 19-27	1.7	11
510	Ferromagnetic Interactions in Highly Stable, Partially Reduced TiO : The S=2 State in Anatase. *Angewandte Chemie - International Edition*, **2017**, 56, 2604-2607	16.4	12
509	Fifty□ifty Zr□i Solid Solution with a TiO2-Type Structure: Electronic Structure and Photochemical Properties of Zirconium Titanate ZrTiO4. *Journal of Physical Chemistry C*, **2017**, 121, 5487-5497	3.8	29
508	Ferromagnetic Interactions in Highly Stable, Partially Reduced TiO2: The S=2 State in Anatase. *Angewandte Chemie*, **2017**, 129, 2648-2651	3.6	2

507	Reducibility of ZrO/PtZr and ZrO/Pt 2D films compared to bulk zirconia: a DFT+U study of oxygen removal and H adsorption. *Nanoscale*, **2017**, 9, 6866-6876	7.7	16
506	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
505	Anchoring Small Au Clusters on the Dehydroxylated and Hydroxylated SiO2 Quartz (001) Surface via Ti-Alloying. *Journal of Physical Chemistry C*, **2017**, 121, 14717-14724	3.8	7
504	HO Adsorption on WO and WO (001) Surfaces. *ACS Applied Materials & Interfaces*, **2017**, 9, 23212-23221	7.5	59
503	CO2 Activation and Hydrogenation: A Comparative DFT Study of Ru10/TiO2 and Cu10/TiO2 Model Catalysts. *Catalysis Letters*, **2017**, 147, 1871-1881	2.8	20
502	Size-dependent dissociation of small cobalt clusters on ultrathin NaCl films. *Nano Research*, **2017**, 10, 1832-1839	10	2
501	Ferromagnetism in nitrogen-doped BaO: a self-interaction corrected DFT study. *Physical Chemistry Chemical Physics*, **2017**, 19, 3279-3286	3.6	7
500	CO Oxidation on Au Nanoparticles Supported on ZrO2: Role of Metal/Oxide Interface and Oxide Reducibility. *ChemCatChem*, **2017**, 9, 1119-1127	5.2	43
499	Reduction of Hydrogenated ZrO Nanoparticles by Water Desorption. *ACS Omega*, **2017**, 2, 3878-3885	3.9	9
498	Increasing Oxide Reducibility: The Role of Metal/Oxide Interfaces in the Formation of Oxygen Vacancies. *ACS Catalysis*, **2017**, 7, 6493-6513	13.1	375
497	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
496	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
495	The photoactive nitrogen impurity in nitrogen-doped zirconium titanate (N-ZrTiO4): a combined electron paramagnetic resonance and density functional theory study. *Journal of Materials Chemistry A*, **2017**, 5, 13062-13071	13	8
494	Adsorption and Dimerization of Late Transition Metal Atoms on the Regular and Defective Quartz (001) Surface. *Topics in Catalysis*, **2017**, 60, 459-470	2.3	10
493	Reprint of Theoretical description of metal/oxide interfacial properties: The case of MgO/Ag(001) *Applied Surface Science*, **2017**, 396, 1850-1854	6.7	
492	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
491	A DFT study of Ni clusters deposition on titania and zirconia (101) surfaces. *Surface Science*, **2016**, 646, 230-238	1.8	20
490	Theoretical description of metal/oxide interfacial properties: The case of MgO/Ag(001). *Applied Surface Science*, **2016**, 390, 578-582	6.7	18

489	Role of Oxide Reducibility in the Deoxygenation of Phenol on Ruthenium Clusters Supported on the Anatase Titania (1 0 1) Surface. *ChemCatChem*, **2016**, 8, 2492-2499	5.2	30
488	Modelling of an ultra-thin silicatene/silicon-carbide hybrid film. *Journal of Physics Condensed Matter* , **2016**, 28, 364005	1.8	2
487	Effect of Nanostructuring on the Reactivity of Zirconia: A DFT+U Study of Au Atom Adsorption. *Journal of Physical Chemistry C*, **2016**, 120, 17604-17612	3.8	10
486	Acetic acid ketonization on tetragonal zirconia: Role of surface reduction. *Journal of Catalysis*, **2016** , 344, 465-473	7.3	35
485	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
484	A DFT study of the acid□base properties of anatase TiO2 and tetragonal ZrO2 by adsorption of CO and CO2 probe molecules. *Surface Science*, **2016**, 652, 163-171	1.8	54
483	Structure and Properties of Zirconia Nanoparticles from Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2016**, 120, 4392-4402	3.8	66
482	CO adsorption on a silica bilayer supported on Ru(0001). *Surface Science*, **2016**, 648, 2-9	1.8	25
481	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
480	Magnetic properties of nitrogen-doped ZrO2: Theoretical evidence of absence of room temperature ferromagnetism. *Scientific Reports*, **2016**, 6, 31435	4.9	18
479	Anisotropic Effects of Oxygen Vacancies on Electrochromic Properties and Conductivity of □Monoclinic WO3. *Journal of Physical Chemistry C*, **2016**, 120, 11716-11726	3.8	59
478	Role of Structural Flexibility on the Physical and Chemical Properties of Metal-Supported Oxide Ultrathin Films. *Springer Series in Materials Science*, **2016**, 91-118	0.9	3
477	Size-Dependent Penetration of Gold Nanoclusters through a Defect-Free, Nonporous NaCl Membrane. *Nano Letters*, **2016**, 16, 3063-70	11.5	12
476	Mechanism of the Cyclo-Oligomerisation of C H on Anatase TiO (101) and (001) Surfaces and Their Reduction: An Electron Paramagnetic Resonance and Density Functional Theory Study. *ChemPlusChem*, **2016**, 81, 64-72	2.8	4
475	Tuning the charge state of Ag and Au atoms and clusters deposited on oxide surfaces by doping: a DFT study of the adsorption properties of nitrogen- and niobium-doped TiO2 and ZrO2. *Physical Chemistry Chemical Physics*, **2015**, 17, 22342-60	3.6	36
474	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
473	Phonon-mediated electron transport through CaO thin films. *Physical Review Letters*, **2015**, 114, 016804	7.4	10
472	Gold and Silver Clusters on TiO2 and ZrO2 (101) Surfaces: Role of Dispersion Forces. *Journal of Physical Chemistry C*, **2015**, 119, 15381-15389	3.8	67

471	Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. *Physical Review B*, **2015**, 91,	3.3	109
470	Numerical Simulations of Defective Structures: The Nature of Oxygen Vacancy in Non-reducible (MgO, SiO2, ZrO2) and Reducible (TiO2, NiO, WO3) Oxides. *Springer Series in Surface Sciences*, **2015**, 1-28	0.4	3
469	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
468	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
467	Characterization of O□Centers on Single Crystalline MgO(001)-Films. *Topics in Catalysis*, **2015**, 58, 811-823	2.3	4
466	DFT Study of CO2Activation on Doped and Ultrathin MgO Films.. *Journal of Physical Chemistry C*, **2015**, 119, 27594-27602	3.8	27
465	Spontaneous doping of two-dimensional NaCl films with Cr atoms: aggregation and electronic structure. *Nanoscale*, **2015**, 7, 2366-73	7.7	9
464	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
463	First Principles Calculations on Oxide-Based Heterogeneous Catalysts and Photocatalysts: Problems and Advances. *Catalysis Letters*, **2015**, 145, 80-94	2.8	45
462	Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. *Journal of Chemical Physics*, **2015**, 143, 134702	3.9	64
461	Communication: Hole localization in Al-doped quartz SiO2 within ab initio hybrid-functional DFT. *Journal of Chemical Physics*, **2015**, 143, 111103	3.9	27
460	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
459	Methanol Oxidation Reaction on □Tungsten Carbide Versus Platinum (1 1 1) Surfaces: A DFT Electrochemical Study. *ChemCatChem*, **2015**, 7, 3533-3543	5.2	13
458	Atomic Scale Structure and Reduction of Cerium Oxide at the Interface with Platinum. *Advanced Materials Interfaces*, **2015**, 2, 1500375	4.6	21
457	Enhanced CO Oxidation on the Oxide/Metal Interface: From Ultra-High Vacuum to Near-Atmospheric Pressures. *ChemCatChem*, **2015**, 7, 2620-2627	5.2	42
456	Lateral manipulation of atomic vacancies in ultrathin insulating films. *ACS Nano*, **2015**, 9, 5318-25	16.7	9
455	Surfaces are different: A perspective on structural, energetic and electronic properties of (001) surfaces of alkaline earth metal oxides as calculated with hybrid density functional theory by Andrew J. Logsdail, David Mora-Fonz, David O. Scanlon, C. Richard A. Catlow, Alexey A. Sokol. *Surface Science*, **2015**, 642, 66-67	1.8	1
454	Nature of Paramagnetic Species in Nitrogen-Doped SnO2: A Combined Electron Paramagnetic Resonance and Density Functional Theory Study. *Journal of Physical Chemistry C*, **2015**, 119, 26895-26903	3.8	16

453	Adsorption of Benzene on Cu(100) and on Cu(100) Covered with an Ultrathin NaCl Film: Molecule–Substrate Interaction and Decoupling. *Journal of Physical Chemistry C*, **2015**, 119, 4062-4071	3.8	17
452	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
451	Cerium-Doped Zirconium Dioxide, a Visible-Light-Sensitive Photoactive Material of Third Generation. *Journal of Physical Chemistry Letters*, **2014**, 5, 447-51	6.4	64
450	Atomistic Modeling of Corrosion Resistance: A First Principles Study of O2 Reduction on the Al(111) Surface Covered with a Thin Hydroxylated Alumina Film. *Advanced Materials Interfaces*, **2014**, 1, 1300072	4.6	34
449	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
448	Properties of two-dimensional insulators: a DFT study of Co adsorption on NaCl and MgO ultrathin films. *Physical Chemistry Chemical Physics*, **2014**, 16, 21838-45	3.6	19
447	Adsorption Properties of Two-Dimensional NaCl: A Density Functional Theory Study of the Interaction of Co, Ag, and Au Atoms with NaCl/Au(111) Ultrathin Films. *Journal of Physical Chemistry C*, **2014**, 118, 12353-12363	3.8	5
446	Ketonization of Carboxylic Acids in Biomass Conversion over TiO2 and ZrO2 Surfaces: A DFT Perspective. *ACS Catalysis*, **2014**, 4, 2874-2888	13.1	112
445	pH Dependent Electronic and Geometric Structures at the Water–Silica Nanoparticle Interface. *Journal of Physical Chemistry C*, **2014**, 118, 29007-29016	3.8	28
444	Nb-doped CaO: an efficient electron donor system. *Journal of Physics Condensed Matter*, **2014**, 26, 315004	2.48	5
443	Carbothermal Transformation of TiO2 into TiOxCy in UHV: Tracking Intrinsic Chemical Stabilities. *Journal of Physical Chemistry C*, **2014**, 118, 22601-22610	3.8	26
442	Adsorption of Li, Na, K, and Mg Atoms on Amorphous and Crystalline Silica Bilayers on Ru(0001): A DFT Study. *Journal of Physical Chemistry C*, **2014**, 118, 15884-15891	3.8	9
441	Two-dimensional oxides and their role in electron transfer mechanisms with adsorbed species. *Chemical Record*, **2014**, 14, 910-22	6.6	7
440	Adsorption of Au and Pd on Ruthenium-Supported Bilayer Silica. *Journal of Physical Chemistry C*, **2014**, 118, 20959-20969	3.8	38
439	Spectroscopic properties of doped and defective semiconducting oxides from hybrid density functional calculations. *Accounts of Chemical Research*, **2014**, 47, 3233-41	24.3	104
438	Identification of Active Sites in a Realistic Model of Strong Metal–Support Interaction Catalysts: The Case of Platinum (1 1 1)-Supported Iron Oxide Film. *ChemCatChem*, **2014**, 6, 185-190	5.2	19
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