Annabella Selloni

List of Publications by Year
in descending order

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205 papers	26,947 citations	6840 81 h-index	6512 162 g-index
210 all docs	210 docs citations	210 times ranked	26395 citing authors

#	Article	IF	Citations
1	Pathways for Electron Transfer at MgOâ€“Water Interfaces from Ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2022, 144, 2002-2009.	6.6	3
2	Structure, Electronic Properties, and Defect Chemistry of Delafossite CuRhO₂ Bulk and Surfaces. Chemistry of Materials, 2022, 34, 1567-1577.	3.2	6
3	Theoretical Insights into Photoelectrochemical Water Reduction on Delafossite CuRhO₂. ACS Energy Letters, 2022, 7, 1528-1533.	8.8	2
4	Structure and Oxygen Evolution Activity of Î²-NiOOH: Where Are the Protons?. ACS Catalysis, 2022, 12, 295-304.	5.5	28
5	Realizing Two-Electron Transfer in Ni(OH)₂ Nanosheets for Energy Storage. Journal of the American Chemical Society, 2022, 144, 8969-8976.	6.6	116
6	Effects of applied voltage on water at a gold electrode interface from ab initio molecular dynamics. Chemical Science, 2021, 12, 5865-5873.	3.7	29
7	Photoexcitation of bulk polarons in rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2021, 103, .	1.1	9
8	Hydration structure of flat and stepped MgO surfaces. Journal of Chemical Physics, 2021, 154, 114708.	1.2	10
9	Polaron-Adsorbate Coupling at the TiO₂(110)-Carboxylate Interface. Journal of Physical Chemistry Letters, 2021, 12, 3571-3576.	2.1	14
10	Conversion of Formic Acid on Single- and Nano-Crystalline Anatase TiO₂(101). Journal of Physical Chemistry C, 2021, 125, 7686-7700.	1.5	10
11	Structure and Reactivity of Pristine and Reduced Spinel CoFe2O4 (001)/(100) Surfaces. Journal of Physical Chemistry C, 2021, 125, 9774-9781.	1.5	8
12	Structure and Stability of Pristine and Carboxylate-Covered Anatase TiO₂(001) in Aqueous Environment. Journal of Physical Chemistry C, 2021, 125, 15910-15917.	1.5	3
13	Hydrogen Bonds and H₃O⁺ Formation at the Water Interface with Formic Acid Covered Anatase TiO₂. Journal of Physical Chemistry Letters, 2021, 12, 6840-6846.	2.1	6
14	Increasing Iridium Oxide Activity for the Oxygen Evolution Reaction with Hafnium Modification. Journal of the American Chemical Society, 2021, 143, 15616-15623.	6.6	82
15	Breaking a dative bond with mechanical forces. Nature Communications, 2021, 12, 5635.	5.8	17
16	Site dependent reactivity of Pt single atoms on anatase TiO₂(101) in an aqueous environment. Physical Chemistry Chemical Physics, 2020, 22, 10455-10461.	1.3	7
17	Methane Activation on Metal-Doped (111) and (100) Ceria Surfaces with Charge-Compensating Oxygen Vacancies. Journal of Physical Chemistry C, 2020, 124, 17578-17585.	1.5	13
18	Oxide chemistry and catalysis. Journal of Chemical Physics, 2020, 153, 050401.	1.2	1

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19	4D Multimodal Nanomedicines Made of Nonequilibrium Auâ€“Fe Alloy Nanoparticles. ACS Nano, 2020, 14, 12840-12853.	7.3	53
20	Binding of Formic Acid on Anatase TiO₂(101). Journal of Physical Chemistry C, 2020, 124, 20228-20239.	1.5	24
21	Theoretical insights into the surface physics and chemistry of redox-active oxides. Nature Reviews Materials, 2020, 5, 460-475.	23.3	89
22	Surface Reactivity of Ag-Modified Ceria to Hydrogen: A Combined Experimental and Theoretical Investigation. ACS Applied Materials & Interfaces, 2020, 12, 27682-27690.	4.0	6
23	Free energy of proton transfer at the waterâ€“TiO₂ interface from ab initio deep potential molecular dynamics. Chemical Science, 2020, 11, 2335-2341.	3.7	134
24	Titania and Its Outstanding Properties: Insights from First Principles Calculations. , 2020, , 29-51.		2
25	Distinct behavior of localized and delocalized carriers in anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> (001) during reaction with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review	0.9	25
26	Structure of disordered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> phases from ab initio based deep neural network simulations. Physical Review Materials, 2020, 4, .	0.9	10
27	Electron Trapping and Ion Leaching at the Li-Modified Quartzâ€“Water Interface. Journal of Physical Chemistry C, 2020, 124, 26741-26747.	1.5	1
28	Versatile Nature of Oxygen Vacancies in Bismuth Vanadate Bulk and (001) Surface. Journal of Physical Chemistry Letters, 2019, 10, 6672-6678.	2.1	32
29	Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO₃ from First Principles. ACS Catalysis, 2019, 9, 10528-10535.	5.5	13
30	Structure and reactivity of highly reduced titanium oxide surface layers on TiO2: A first-principles study. Journal of Chemical Physics, 2019, 151, 184701.	1.2	7
31	Preface to Special Issue of ChemSusChemâ€”Water Splitting: From Theory to Practice. ChemSusChem, 2019, 12, 1771-1774.	3.6	7
32	H₂ Dissociation on Noble Metal Single Atom Catalysts Adsorbed on and Doped into CeO₂ (111). Journal of Physical Chemistry C, 2019, 123, 9875-9883.	1.5	33
33	Structure and stability of NaTaO3(001) and KTaO3(001) surfaces. Physical Review Materials, 2019, 3, .	0.9	16
34	Electronic and optical properties of doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> by many-body perturbation theory. Physical Review Materials, 2019, 3, .	0.9	28
35	Excess electrons in reduced rutile and anatase TiO2. Surface Science Reports, 2018, 73, 58-82.	3.8	106
36	Stable Hydrogen Evolution from an AgRhO₂ Photocathode under Visible Light. Chemistry of Materials, 2018, 30, 2574-2582.	3.2	19

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37	Effect of Structural Fluctuations on Elastic Lifetimes of Adsorbate States: Isonicotinic Acid on Rutile(110). Journal of Physical Chemistry C, 2018, 122, 7575-7585.	1.5	7
38	Structure, Polarization, and Sum Frequency Generation Spectrum of Interfacial Water on Anatase TiO₂. Journal of Physical Chemistry Letters, 2018, 9, 6716-6721.	2.1	70
39	Defects, Adsorbates, and Photoactivity of Rutile TiO₂ (110): Insight by First-Principles Calculations. Journal of Physical Chemistry Letters, 2018, 9, 5281-5287.	2.1	33
40	Water Dissociates at the Aqueous Interface with Reduced Anatase TiO₂ (101). Journal of Physical Chemistry Letters, 2018, 9, 3131-3136.	2.1	45
41	Electronic structure and photoabsorption of Ti³⁺ ions in reduced anatase and rutile TiO₂. Physical Chemistry Chemical Physics, 2018, 20, 17658-17665.	1.3	38
42	Titania and Its Outstanding Properties: Insights from First Principles Calculations. , 2018, , 1-23.		1
43	Self-hydrogenated shell promoting photocatalytic H2 evolution on anatase TiO2. Nature Communications, 2018, 9, 2752.	5.8	178
44	Structural evolution of titanium dioxide during reduction in high-pressure hydrogen. Nature Materials, 2018, 17, 923-928.	13.3	100
45	Mechanism and activity of CO oxidation on (001) and (110) surfaces of spinel Co3O4, NiCo2O4 and NiFe2O4: A DFTâ€ +â€U study. Surface Science, 2018, 677, 278-283.	0.8	18
46	Influence of Bulky Organoâ€Ammonium Halide Additive Choice on the Flexibility and Efficiency of Perovskite Lightâ€Emitting Devices. Advanced Functional Materials, 2018, 28, 1802060.	7.8	76
47	Formation and stability of reduced <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math> layers on anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mn>101</mml:mn>	0.9	11
48	Effects of Alkali Cations and Sulfate/Chloride Anions on the Flux Growth of {001}-Faceted Î²-Li₂TiO₃ Crystals. Crystal Growth and Design, 2017, 17, 1118-1124.	1.4	17
49	Oxygen Deficiency and Reactivity of Spinel NiCo₂O₄ (001) Surfaces. Journal of Physical Chemistry C, 2017, 121, 3929-3937.	1.5	39
50	Geometric structure of anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mn>101</mml:mn> Physical Review B, 2017, 95, .	1.1	45
51	Formaldehyde Adsorption on the Anatase TiO₂(101) Surface: Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2017, 121, 8914-8922.	1.5	32
52	Effect of reducible oxideâ€“metal cluster charge transfer on the structure and reactivity of adsorbed Au and Pt atoms and clusters on anatase TiO2. Journal of Chemical Physics, 2017, 146, .	1.2	18
53	Excess electrons at anatase TiO₂surfaces and interfaces: insights from first principles simulations. Journal Physics D: Applied Physics, 2017, 50, 273002.	1.3	16
54	Surface Structure of TiO₂ Rutile (011) Exposed to Liquid Water. Journal of Physical Chemistry C, 2017, 121, 26424-26431.	1.5	37

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55	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	3.3	340
56	Methanol on Anatase TiO₂ (101): Mechanistic Insights into Photocatalysis. ACS Catalysis, 2017, 7, 7081-7091.	5.5	93
57	The Reactivity of Anatase TiO2 (211) Surface and the Bond- Charge Counting Model. , 2017, , .		2
58	Following the Reduction of Oxygen on TiO₂ Anatase (101) Step by Step. Journal of the American Chemical Society, 2016, 138, 9565-9571.	6.6	74
59	Platy KTiNbO5 as a Selective Sr Ion Adsorbent: Crystal Growth, Adsorption Experiments, and DFT Calculations. Journal of Physical Chemistry C, 2016, 120, 11984-11992.	1.5	15
60	Ab Initio Simulation of the Absorption Spectra of Photoexcited Carriers in TiO₂ Nanoparticles. Journal of Physical Chemistry Letters, 2016, 7, 3597-3602.	2.1	23
61	AbÂInitioStudy of Water Adsorption and Reactivity on the (211) Surface of Anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> Physical Review Applied, 2016, 5, .	1.5	12
62	Pathway of Photocatalytic Oxygen Evolution on Aqueous TiO₂ Anatase and Insights into the Different Activities of Anatase and Rutile. ACS Catalysis, 2016, 6, 4769-4774.	5.5	76
63	Facet-dependent trapping and dynamics of excess electrons at anatase TiO2 surfaces and aqueous interfaces. Nature Materials, 2016, 15, 1107-1112.	13.3	303
64	Formation, Electronic Structure, and Defects of Ni Substituted Spinel Cobalt Oxide: a DFT+U Study. Journal of Physical Chemistry C, 2016, 120, 14892-14898.	1.5	86
65	Real-Time Observation of Reconstruction Dynamics on TiO₂(001) Surface under Oxygen via an Environmental Transmission Electron Microscope. Nano Letters, 2016, 16, 132-137.	4.5	109
66	Effects of Thermal Fluctuations on the Structure, Level Alignment, and Absorption Spectrum of Dye-Sensitized TiO₂: A Comparative Study of Catechol and Isonicotinic Acid on the Anatase (101) and Rutile (110) Surfaces. Journal of Physical Chemistry C, 2016, 120, 3899-3905.	1.5	12
67	Structural and Electronic Properties of Photoexcited TiO₂ Nanoparticles from First Principles. Journal of Chemical Theory and Computation, 2015, 11, 635-645.	2.3	32
68	Combined Effects of Functional Groups, Lattice Defects, and Edges in the Infrared Spectra of Graphene Oxide. Journal of Physical Chemistry C, 2015, 119, 18167-18176.	1.5	134
69	Localized Excitation of Ti³⁺ Ions in the Photoabsorption and Photocatalytic Activity of Reduced Rutile TiO₂. Journal of the American Chemical Society, 2015, 137, 9146-9152.	6.6	168
70	DFT+U Study of the Surface Structure and Stability of Co₃O₄(110): Dependence on U. Journal of Physical Chemistry C, 2015, 119, 9973-9979.	1.5	107
71	Ab initio simulations of the structure of thin water layers on defective anatase <scp>T</scp><scp>O</scp>₂(101) surfaces. International Journal of Quantum Chemistry, 2015, 115, 1250-1257.	1.0	20
72	A Multitechnique Study of CO Adsorption on the TiO₂ Anatase (101) Surface. Journal of Physical Chemistry C, 2015, 119, 21044-21052.	1.5	59

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73	Adsorption of biomedical coating molecules, amino acids, and short peptides on magnetite (110). Journal of Chemical Physics, 2015, 143, 044705.	1.2	22
74	Structure of the NiFe2O4(001) surface in contact with gaseous O2 and water vapor. Surface Science, 2015, 640, 73-79.	0.8	30
75	Mosaic Texture and Doublec-Axis Periodicity of Î²-NiOOH: Insights from First-Principles and Genetic Algorithm Calculations. Journal of Physical Chemistry Letters, 2014, 5, 3981-3985.	2.1	65
76	Identification of adsorbed molecules via STM tip manipulation: CO, H₂O, and O₂ on TiO₂ anatase (101). Physical Chemistry Chemical Physics, 2014, 16, 21524-21530.	1.3	48
77	Influence of external electric fields on oxygen vacancies at the anatase (101) surface. Journal of Chemical Physics, 2014, 141, 084705.	1.2	22
78	Introduction: Titanium Dioxide (TiO₂) Nanomaterials. Chemical Reviews, 2014, 114, 9281-9282.	23.0	370
79	Theoretical Studies on Anatase and Less Common TiO₂ Phases: Bulk, Surfaces, and Nanomaterials. Chemical Reviews, 2014, 114, 9708-9753.	23.0	367
80	Mechanism and Activity of Water Oxidation on Selected Surfaces of Pure and Fe-Doped NiO_x. ACS Catalysis, 2014, 4, 1148-1153.	5.5	403
81	TiO2 /Ferroelectric Heterostructures as Dynamic Polarization-Promoted Catalysts for Photochemical and Electrochemical Oxidation of Water. Physical Review Letters, 2014, 112, 196102.	2.9	63
82	Adsorption and Reactions of O₂ on Anatase TiO₂. Accounts of Chemical Research, 2014, 47, 3361-3368.	7.6	140
83	Evolution of nanostructures of anatase TiO2 thin films grown on (001) LaAlO3. Journal of Nanoparticle Research, 2013, 15, 1.	0.8	10
84	Reaction of O ₂ with Subsurface Oxygen Vacancies on TiO ₂ Anatase (101). Science, 2013, 341, 988-991.	6.0	474
85	Oxygen tolerance of an in silico -designed bioinspired hydrogen-evolving catalyst in water. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 2017-2022.	3.3	6
86	Inherent electronic trap states in TiO2 nanocrystals: effect of saturation and sintering. Energy and Environmental Science, 2013, 6, 1221.	15.6	76
87	Surface Structure and Reactivity of Anatase TiO₂ Crystals with Dominant {001} Facets. Journal of Physical Chemistry C, 2013, 117, 6358-6362.	1.5	85
88	Theoretical Study of Interfacial Electron Transfer from Reduced Anatase TiO₂(101) to Adsorbed O₂. Journal of the American Chemical Society, 2013, 135, 9195-9199.	6.6	90
89	Directional Heat Dissipation across the Interface in Anataseâ€“Rutile Nanocomposites. ACS Applied Materials & Interfaces, 2013, 5, 9883-9890.	4.0	79
90	First Principles Study of Cobalt (Hydr)oxides under Electrochemical Conditions. Journal of Physical Chemistry C, 2013, 117, 20002-20006.	1.5	89

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91	Chemical Dynamics of the First Proton-Coupled Electron Transfer of Water Oxidation on TiO₂ Anatase. Journal of the American Chemical Society, 2013, 135, 18774-18777.	6.6	147
92	Enhanced Thermal Decomposition of Nitromethane on Functionalized Graphene Sheets: Ab Initio Molecular Dynamics Simulations. Journal of the American Chemical Society, 2012, 134, 19011-19016.	6.6	83
93	DFT-GGA and DFT+U Simulations of Thin Water Layers on Reduced TiO₂ Anatase. Journal of Physical Chemistry C, 2012, 116, 9114-9121.	1.5	56
94	(Sub)Surface Mobility of Oxygen Vacancies at the<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>Anatase (101) Surface. Physical Review Letters, 2012, 109, 136103.	2.9	176
95	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>(110) surface: A first-principles study. Physical Review B, 2012, 85, .	1.1	95
96	Water Adsorption and Oxidation at the Co₃O₄ (110) Surface. Journal of Physical Chemistry Letters, 2012, 3, 2808-2814.	2.1	97
97	Interaction of Oxygen and Water with the (100) Surface of Pyrite: Mechanism of Sulfur Oxidation. Journal of Physical Chemistry Letters, 2012, 3, 2409-2414.	2.1	76
98	Hydrogen interaction with the anatase TiO2(101) surface. Physical Chemistry Chemical Physics, 2012, 14, 16595.	1.3	104
99	Solvent Effects on the Adsorption Geometry and Electronic Structure of Dye-Sensitized TiO₂: A First-Principles Investigation. Journal of Physical Chemistry C, 2012, 116, 5932-5940.	1.5	83
100	Interaction of Water with the Fluorine-Covered Anatase TiO₂ (001) Surface. Journal of Physical Chemistry C, 2011, 115, 17092-17096.	1.5	21
101	Hydrogen Incorporation and Storage in Well-Defined Nanocrystals of Anatase Titanium Dioxide. Journal of Physical Chemistry C, 2011, 115, 25590-25594.	1.5	93
102	Electronic structure and bonding properties of cobalt oxide in the spinel structure. Physical Review B, 2011, 83, .	1.1	258
103	Growth and Organization of an Organic Molecular Monolayer on TiO₂: Catechol on Anatase (101). Journal of the American Chemical Society, 2011, 133, 7816-7823.	6.6	106
104	Simple, Unambiguous Theoretical Approach to Oxidation State Determination via First-Principles Calculations. Inorganic Chemistry, 2011, 50, 10259-10267.	1.9	103
105	Bulk and Surface Polarons in Photoexcited Anatase TiO₂. Journal of Physical Chemistry Letters, 2011, 2, 2223-2228.	2.1	232
106	Oxidation State Changes and Electron Flow in Enzymatic Catalysis and Electrocatalysis through Wannierâ€Function Analysis. Chemistry - A European Journal, 2011, 17, 12136-12143.	1.7	30
107	Electrocatalyst design from first principles: A hydrogen-production catalyst inspired by nature. Catalysis Today, 2011, 165, 160-170.	2.2	6
108	Titania-water interactions: a review of theoretical studies. Journal of Materials Chemistry, 2010, 20, 10319.	6.7	255

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109	Theoretical Design by First Principles Molecular Dynamics of a Bioinspired Electrodeâ^'Catalyst System for Electrocatalytic Hydrogen Production from Acidified Water. Journal of Chemical Theory and Computation, 2010, 6, 3490-3502.	2.3	14
110	Influence of Subsurface Defects on the Surface Reactivity of TiO₂: Water on Anatase (101). Journal of Physical Chemistry C, 2010, 114, 1278-1284.	1.5	206
111	Surface Radical Chain Reaction Revisited: Comparative Investigation of Styrene and 2,4-Dimethyl-Styrene on Hydrogenated Si(001) Surface from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2010, 114, 3981-3986.	1.5	22
112	First-Principles Modeling of the Adsorption Geometry and Electronic Structure of Ru(II) Dyes on Extended TiO₂ Substrates for Dye-Sensitized Solar Cell Applications. Journal of Physical Chemistry C, 2010, 114, 6054-6061.	1.5	224
113	Simulation of Electrocatalytic Hydrogen Production by a Bioinspired Catalyst Anchored to a Pyrite Electrode. Journal of the American Chemical Society, 2010, 132, 8593-8601.	6.6	33
114	Hydroxide Ions at the Water/Anatase TiO2(101) Interface: Structure and Electronic States from First Principles Molecular Dynamics. Langmuir, 2010, 26, 11518-11525.	1.6	76
115	Peroxide and superoxide states of adsorbed O2 on anatase TiO2 (101) with subsurface defects. Physical Chemistry Chemical Physics, 2010, 12, 12956.	1.3	132
116	Hydroxylation of TiO2-B: insights from density functional calculations. Journal of Materials Chemistry, 2010, 20, 5871.	6.7	17
117	Evidence for the Predominance of Subsurface Defects on Reduced Anatase<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:mo stretchy="false">(</mml:mo><mml:mn>101</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 407 Td (stretchy="fa	2.9	232
118	Order-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>implementation of exact exchange in extended insulating systems. Physical Review B, 2009, 79, .	1.1	171
119	The 2Ã—1 reconstruction of the rutile TiO2(011) surface: A combined density functional theory, X-ray diffraction, and scanning tunneling microscopy study. Surface Science, 2009, 603, 138-144.	0.8	99
120	Local ordering and electronic signatures of submonolayer water on anatase TiO2(101). Nature Materials, 2009, 8, 585-589.	13.3	298
121	Hydrogen Production by the Naked Active Site of the Di-iron Hydrogenases in Water. Journal of Physical Chemistry B, 2009, 113, 13096-13106.	1.2	10
122	Reduced and n-Type Doped TiO₂: Nature of Ti³⁺ Species. Journal of Physical Chemistry C, 2009, 113, 20543-20552.	1.5	652
123	Nucleation and Growth of 1D Water Clusters on Rutile TiO₂(011)-2Ã—1. Journal of Physical Chemistry C, 2009, 113, 10329-10332.	1.5	33
124	Correlation between Bonding Geometry and Band Gap States at Organicâ^'Inorganic Interfaces: Catechol on Rutile TiO₂(110). Journal of the American Chemical Society, 2009, 131, 980-984.	6.6	169
125	First Principles Study of Fatty Acid Monolayers on Au(111)^{â€}. Journal of Physical Chemistry C, 2009, 113, 8895-8900.	1.5	28
126	Hybrid density functional calculations of the band gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ga</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> Physical Review B, 2009, 80, .	1.1	41

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127	First Principles Study of Hydrated/Hydroxylated TiO₂ Nanolayers: From Isolated Sheets to Stacks and Tubes. ACS Nano, 2009, 3, 317-324.	7.3	47
128	Structure and Stability of TiO₂-B Surfaces: A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 18973-18977.	1.5	67
129	Surface and subsurface oxygen vacancies in anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> differences with rutile. Physical Review B, 2009, 79, .	1.1	274
130	Alignment of the dyeâ€™s molecular levels with the TiO₂band edges in dye-sensitized solar cells: a DFTâ€“TDDFT study. Nanotechnology, 2008, 19, 424002.	1.3	263
131	Anatase shows its reactive side. Nature Materials, 2008, 7, 613-615.	13.3	472
132	Different Reactivities of TiO₂ Polymorphs:â€‰ Comparative DFT Calculations of Water and Formic Acid Adsorption at Anatase and Brookite TiO₂ Surfaces. Journal of Physical Chemistry C, 2008, 112, 6594-6596.	1.5	102
133	Small Au and Pt Clusters at the Anatase TiO₂(101) Surface:â€‰ Behavior at Terraces, Steps, and Surface Oxygen Vacancies. Journal of the American Chemical Society, 2008, 130, 370-381.	6.6	276
134	Mechanism of H₂ Production by the [FeFe]_H Subcluster of Di-Iron Hydrogenases: Implications for Abiotic Catalysts. Journal of Physical Chemistry B, 2008, 112, 13381-13390.	1.2	12
135	Excess electron states in reduced bulk anatase TiO2: Comparison of standard GGA, GGA+U, and hybrid DFT calculations. Journal of Chemical Physics, 2008, 129, 154113.	1.2	472
136	Band alignment in molecular devices: Influence of anchoring group and metal work function. Physical Review B, 2008, 77, .	1.1	33
137	The c(4 Ã— 2) Structure of Short- and Intermediate-Chain Length Alkanethiolate Monolayers on Au(111):â€‰ A DFT Study. Journal of Physical Chemistry C, 2007, 111, 12149-12151.	1.5	54
138	Influence of End Group and Surface Structure on the Currentâˆ’Voltage Characteristics of Alkanethiol Monolayers on Au(111). Journal of Physical Chemistry A, 2007, 111, 12381-12385.	1.1	16
139	Viewpoint: Chemistry for a Sustainable Future. Environmental Science & Technology, 2007, 41, 4840-4846.	4.6	32
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