

# Livia Giordano

## List of Publications by Year in descending order

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165  
papers

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docs citations

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times ranked

14949  
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#	ARTICLE	IF	CITATIONS
1	Electronic Structure-Based Descriptors for Oxide Properties and Functions. <i>Accounts of Chemical Research</i> , 2022, 55, 298-308.	7.6	42
2	Implications of Nonelectrochemical Reaction Steps on the Oxygen Evolution Reaction: Oxygen Dimer Formation on Perovskite Oxide and Oxynitride Surfaces. <i>ACS Catalysis</i> , 2022, 12, 1433-1442.	5.5	12
3	Tunable metal hydroxide-organic frameworks for catalysing oxygen evolution. <i>Nature Materials</i> , 2022, 21, 673-680.	13.3	123
4	Surface Oxygen Vacancies Confined by Ferroelectric Polarization for Tunable CO Oxidation Kinetics. <i>Advanced Materials</i> , 2022, 34, e2202072.	11.1	13
5	Molecularly Tunable Polyanions for Single-Ion Conductors and Poly(solvate ionic liquids). <i>Chemistry of Materials</i> , 2021, 33, 524-534.	3.2	53
6	Towards controlling the reversibility of anionic redox in transition metal oxides for high-energy Li-ion positive electrodes. <i>Energy and Environmental Science</i> , 2021, 14, 2322-2334.	15.6	41
7	Regulating oxygen activity of perovskites to promote NO <sub>x</sub> oxidation and reduction kinetics. <i>Nature Catalysis</i> , 2021, 4, 663-673.	16.1	54
8	Cation- and pH-Dependent Hydrogen Evolution and Oxidation Reaction Kinetics. <i>Jacs Au</i> , 2021, 1, 1674-1687.	3.6	109
9	Enhancing oxygen reduction electrocatalysis by tuning interfacial hydrogen bonds. <i>Nature Catalysis</i> , 2021, 4, 753-762.	16.1	122
10	Direct Observation of Surface-Bound Intermediates During Methanol Oxidation on Platinum Under Alkaline Conditions. <i>Journal of Physical Chemistry C</i> , 2021, 125, 26321-26331.	1.5	8
11	Revealing electrolyte oxidation <i>via</i> carbonate dehydrogenation on Ni-based oxides in Li-ion batteries by <i>in situ</i> Fourier transform infrared spectroscopy. <i>Energy and Environmental Science</i> , 2020, 13, 183-199.	15.6	202
12	Conversion of Methane into Liquid Fuels—Bridging Thermal Catalysis with Electrocatalysis. <i>Advanced Energy Materials</i> , 2020, 10, 2002154.	10.2	57
13	Probing Depth-Dependent Transition-Metal Redox of Lithium Nickel, Manganese, and Cobalt Oxides in Li-Ion Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 55865-55875.	4.0	14
14	Operando identification of site-dependent water oxidation activity on ruthenium dioxide single-crystal surfaces. <i>Nature Catalysis</i> , 2020, 3, 516-525.	16.1	166
15	Toward Establishing Electronic and Phononic Signatures of Reversible Lattice Oxygen Oxidation in Lithium Transition Metal Oxides For Li-Ion Batteries. <i>Chemistry of Materials</i> , 2020, 32, 5502-5514.	3.2	17
16	The Role of Diphenyl Carbonate Additive on the Interfacial Reactivity of Positive Electrodes in Li-ion Batteries. <i>Journal of the Electrochemical Society</i> , 2020, 167, 040522.	1.3	8
17	Bismuth Substituted Strontium Cobalt Perovskites for Catalyzing Oxygen Evolution. <i>Journal of Physical Chemistry C</i> , 2020, 124, 6562-6570.	1.5	41
18	Design of S-Substituted Fluorinated Aryl Sulfonamide-Tagged (S-FAST) Anions To Enable New Solvate Ionic Liquids for Battery Applications. <i>Chemistry of Materials</i> , 2019, 31, 7558-7564.	3.2	11

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19	Enhanced Cycling Performance of Ni-Rich Positive Electrodes (NMC) in Li-Ion Batteries by Reducing Electrolyte Free-Solvent Activity. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 34973-34988.	4.0	63
20	Ligand-Dependent Energetics for Dehydrogenation: Implications in Li-Ion Battery Electrolyte Stability and Selective Oxidation Catalysis of Hydrogen-Containing Molecules. <i>Chemistry of Materials</i> , 2019, 31, 5464-5474.	3.2	28
21	Revealing Electronic Signatures of Lattice Oxygen Redox in Lithium Ruthenates and Implications for High-Energy Li-Ion Battery Material Designs. <i>Chemistry of Materials</i> , 2019, 31, 7864-7876.	3.2	47
22	Editors' Choice "Coating-Dependent Electrode-Electrolyte Interface for Ni-Rich Positive Electrodes in Li-Ion Batteries. <i>Journal of the Electrochemical Society</i> , 2019, 166, A1022-A1030.	1.3	41
23	An <i>In Situ</i> Surface-Enhanced Infrared Absorption Spectroscopy Study of Electrochemical CO <sub>2</sub> Reduction: Selectivity Dependence on Surface C-Bound and O-Bound Reaction Intermediates. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5951-5963.	1.5	172
24	The Effect of Electrode-Electrolyte Interface on the Electrochemical Impedance Spectra for Positive Electrode in Li-Ion Battery. <i>Journal of the Electrochemical Society</i> , 2019, 166, A5090-A5098.	1.3	190
25	Tuning mobility and stability of lithium ion conductors based on lattice dynamics. <i>Energy and Environmental Science</i> , 2018, 11, 850-859.	15.6	158
26	Oxidation of Ethylene Carbonate on Li Metal Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10442-10449.	1.5	60
27	Iron-Based Perovskites for Catalyzing Oxygen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8445-8454.	1.5	106
28	Fluorinated Aryl Sulfonimide Tagged (FAST) salts: modular synthesis and structure-property relationships for battery applications. <i>Energy and Environmental Science</i> , 2018, 11, 1326-1334.	15.6	26
29	Coupled LiPF <sub>6</sub> Decomposition and Carbonate Dehydrogenation Enhanced by Highly Covalent Metal Oxides in High-Energy Li-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27368-27382.	1.5	127
30	Surface (Electro)chemistry of CO <sub>2</sub> on Pt Surface: An <i>In Situ</i> Surface-Enhanced Infrared Absorption Spectroscopy Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12341-12349.	1.5	19
31	Terrace site hydroxylation upon water dimer formation on monolayer NiO/Ag(100). <i>Thin Solid Films</i> , 2018, 660, 365-372.	0.8	4
32	Lithium Conductivity and Meyer-Neldel Rule in Li <sub>3</sub> PO <sub>4</sub> -Li <sub>3</sub> VO <sub>4</sub> -Li <sub>4</sub> GeO <sub>4</sub> Lithium Superionic Conductors. <i>Chemistry of Materials</i> , 2018, 30, 5573-5582.	3.2	74
33	Surface Orientation Dependent Water Dissociation on Rutile Ruthenium Dioxide. <i>Journal of Physical Chemistry C</i> , 2018, 122, 17802-17811.	1.5	44
34	Probing Surface Chemistry Changes Using LiCoO <sub>2</sub> -only Electrodes in Li-Ion Batteries. <i>Journal of the Electrochemical Society</i> , 2018, 165, A1377-A1387.	1.3	46
35	Activating lattice oxygen redox reactions in metal oxides to catalyse oxygen evolution. <i>Nature Chemistry</i> , 2017, 9, 457-465.	6.6	1,409
36	Mapping a stable solvent structure landscape for aprotic Li-air battery organic electrolytes. <i>Journal of Materials Chemistry A</i> , 2017, 5, 23987-23998.	5.2	33

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37	In Situ Spectroscopy and Mechanistic Insights into CO Oxidation on Transition-Metal-Substituted Ceria Nanoparticles. <i>ACS Catalysis</i> , 2017, 7, 6843-6857.	5.5	78
38	Chemical Reactivity Descriptor for the Oxide-Electrolyte Interface in Li-Ion Batteries. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3881-3887.	2.1	104
39	Towards identifying the active sites on RuO <sub>2</sub> (110) in catalyzing oxygen evolution. <i>Energy and Environmental Science</i> , 2017, 10, 2626-2637.	15.6	278
40	Perovskites in catalysis and electrocatalysis. <i>Science</i> , 2017, 358, 751-756.	6.0	1,138
41	Reprint of "Theoretical description of metal/oxide interfacial properties: The case of MgO/Ag(001)". <i>Applied Surface Science</i> , 2017, 396, 1850-1854.	3.1	0
42	Charge-transfer-energy-dependent oxygen evolution reaction mechanisms for perovskite oxides. <i>Energy and Environmental Science</i> , 2017, 10, 2190-2200.	15.6	401
43	Activity and stability of cobalt phosphides for hydrogen evolution upon water splitting. <i>Nano Energy</i> , 2016, 29, 37-45.	8.2	166
44	Correlation of nanoscale behaviour of forces and macroscale surface wettability. <i>Nanoscale</i> , 2016, 8, 15597-15603.	2.8	23
45	The effect of water on discharge product growth and chemistry in Li <sup>+</sup> O <sub>2</sub> batteries. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24944-24953.	1.3	73
46	Water dissociation on MnO(1 $\bar{1}$ )/Ag(100). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25355-25363.	1.3	7
47	Theoretical description of metal/oxide interfacial properties: The case of MgO/Ag(001). <i>Applied Surface Science</i> , 2016, 390, 578-582.	3.1	21
48	The effect of oxygen vacancies on water wettability of transition metal based SrTiO <sub>3</sub> and rare-earth based Lu <sub>2</sub> O <sub>3</sub> . <i>RSC Advances</i> , 2016, 6, 109234-109240.	1.7	40
49	Elucidating the Nature of the Active Phase in Copper/Ceria Catalysts for CO Oxidation. <i>ACS Catalysis</i> , 2016, 6, 1675-1679.	5.5	122
50	Inorganic Solid-State Electrolytes for Lithium Batteries: Mechanisms and Properties Governing Ion Conduction. <i>Chemical Reviews</i> , 2016, 116, 140-162.	23.0	1,777
51	pH dependence of OER activity of oxides: Current and future perspectives. <i>Catalysis Today</i> , 2016, 262, 2-10.	2.2	288
52	Atomic Scale Structure and Reduction of Cerium Oxide at the Interface with Platinum. <i>Advanced Materials Interfaces</i> , 2015, 2, 1500375.	1.9	25
53	Enhanced CO Oxidation on the Oxide/Metal Interface: From Ultra-High Vacuum to Near-Atmospheric Pressures. <i>ChemCatChem</i> , 2015, 7, 2620-2627.	1.8	47
54	Reactivity of Perovskites with Water: Role of Hydroxylation in Wetting and Implications for Oxygen Electrocatalysis. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18504-18512.	1.5	88

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55	Electrode-Electrolyte Interface in Li-Ion Batteries: Current Understanding and New Insights. Journal of Physical Chemistry Letters, 2015, 6, 4653-4672.	2.1	811
56	Spontaneous Oxidation of Ni Nanoclusters on MgO Monolayers Induced by Segregation of Interfacial Oxygen. Journal of Physical Chemistry Letters, 2015, 6, 3104-3109.	2.1	15
57	Identification of Active Sites in a Realistic Model of Strong Metal-Support Interaction Catalysts: The Case of Platinum(111)-Supported Iron Oxide Film. ChemCatChem, 2014, 6, 185-190.	1.8	19
58	Surface defects and their impact on the electronic structure of Mo-doped CaO films: an STM and DFT study. Physical Chemistry Chemical Physics, 2014, 16, 12764-12772.	1.3	19
59	Self-Doping of Ultrathin Insulating Films by Transition Metal Atoms. Physical Review Letters, 2014, 112, 026102.	2.9	23
60	Properties of Pt-supported iron oxide ultra-thin films: Similarity of Hubbard-corrected and hybrid density functional theory description. Journal of Chemical Physics, 2014, 141, 144702.	1.2	19
61	Structure, Bonding, and Catalytic Activity of Monodisperse, Transition-Metal-Substituted CeO <sub>2</sub> Nanoparticles. Journal of the American Chemical Society, 2014, 136, 17193-17200.	6.6	149
62	Understanding surface core-level shifts using the Auger parameter: A study of Pd atoms adsorbed on ultrathin SiO <sub>2</sub> films. Physical Review B, 2014, 89, .	1.1	38
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.	1.5	31
64	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.	1.5	7
65	pH Dependent Electronic and Geometric Structures at the Water-Silica Nanoparticle Interface. Journal of Physical Chemistry C, 2014, 118, 29007-29016.	1.5	32
66	Nb-doped CaO: an efficient electron donor system. Journal of Physics Condensed Matter, 2014, 26, 315004.	0.7	5
67	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.	1.5	13
68	Adsorption of Au and Pd on Ruthenium-Supported Bilayer Silica. Journal of Physical Chemistry C, 2014, 118, 20959-20969.	1.5	46
69	Spectroscopic Evidences of Charge Transfer Phenomena and Stabilization of Unusual Phases at Iron Oxide Monolayers Grown on Pt(111). Topics in Catalysis, 2013, 56, 1074-1081.	1.3	11
70	Charging of Gold Atoms on Doped MgO and CaO: Identifying the Key Parameters by DFT Calculations. Journal of Physical Chemistry C, 2013, 117, 9943-9951.	1.5	45
71	From Heterolytic to Homolytic H <sub>2</sub> Dissociation on Nanostructured MgO(001) Films As a Function of the Metal Support. Journal of Physical Chemistry C, 2013, 117, 10623-10629.	1.5	57
72	Polarity compensation in low-dimensional oxide nanostructures: The case of metal-supported MgO nanoribbons. Physical Review B, 2013, 87, .	1.1	16

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73	Controlling the charge state of single Mo dopants in a CaO film. <i>Physical Review B</i> , 2013, 88, .	1.1	24
74	Electronic and electrostatic properties of polar oxide nanostructures: MgO(111) islands on Au(111). <i>Physical Review B</i> , 2012, 86, .	1.1	20
75	Li, Al, and Ni Substitutional Doping in MgO Ultrathin Films on Metals: Work Function Tuning via Charge Compensation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5781-5786.	1.5	30
76	Tuning the Charge State of (WO <sub>3</sub> ) <sub>3</sub> Nanoclusters Deposited on MgO/Ag(001) Films. <i>Journal of Physical Chemistry C</i> , 2012, 116, 17668-17675.	1.5	18
77	Modified Ion Pair Interaction for Water Dimers on Supported MgO Ultrathin Films. <i>Journal of Physical Chemistry C</i> , 2012, 116, 20349-20355.	1.5	19
78	Resolving all atoms of an alkali halide via nanomodulation of the thin NaCl film surface using the Au(111) reconstruction. <i>Physical Review B</i> , 2012, 85, .	1.1	33
79	Donor Characteristics of Transition-Metal-Doped Oxides: Cr-Doped MgO versus Mo-Doped CaO. <i>Journal of the American Chemical Society</i> , 2012, 134, 11380-11383.	6.6	90
80	Compensating Edge Polarity: A Means To Alter the Growth Orientation of MgO Nanostructures on Au(111). <i>Journal of Physical Chemistry C</i> , 2012, 116, 11126-11132.	1.5	15
81	Interaction of Water with FeO(111)/Pt(111): Environmental Effects and Influence of Oxygen. <i>Journal of Physical Chemistry C</i> , 2011, 115, 19328-19335.	1.5	39
82	Density functional theory study of TiO <sub>2</sub> /Ag interfaces and their role in memristor devices. <i>Physical Review B</i> , 2011, 83, .	1.1	43
83	Oxide Films at the Nanoscale: New Structures, New Functions, and New Materials. <i>Accounts of Chemical Research</i> , 2011, 44, 1244-1252.	7.6	156
84	CO+NO versus CO+O <sub>2</sub> Reaction on Monolayer FeO(111) Films on Pt(111). <i>ChemCatChem</i> , 2011, 3, 671-674.	1.8	29
85	Activation of Oxygen on MgO: O <sub>2</sub> <sup>•-</sup> Radical Ion Formation on Thin, Metal-Supported MgO(001) Films. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 2635-2638.	7.2	101
86	Tailoring the Shape of Metal Ad-Particles by Doping the Oxide Support. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11525-11527.	7.2	99
87	Strain-induced formation of ultrathin mixed-oxide films. <i>Physical Review B</i> , 2011, 83, .	1.1	34
88	Mechanism of Charging of Au Atoms and Nanoclusters on Li Doped SiO <sub>2</sub> /Mo(112) Films. <i>ChemPhysChem</i> , 2010, 11, 412-418.	1.0	14
89	The Interplay between Structure and CO Oxidation Catalysis on Metal-Supported Ultrathin Oxide Films. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 4418-4421.	7.2	191
90	Polarity of ultrathin MgO(111) films deposited on a metal substrate. <i>Physical Review B</i> , 2010, 81, .	1.1	25

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91	Oxygen-Induced Transformations of an FeO(111) Film on Pt(111): A Combined DFT and STM Study. Journal of Physical Chemistry C, 2010, 114, 21504-21509.	1.5	90
92	Stabilizing Monomeric Iron Species in a Porous Silica/Mo(112) Film. ACS Nano, 2010, 4, 863-868.	7.3	11
93	Direct Measurement of the Attractive Interaction Forces on F <sup>0</sup> Color Centers on MgO(001) by Dynamic Force Microscopy. ACS Nano, 2010, 4, 2510-2514.	7.3	29
94	Zero-bias conductance anomaly of a FeO-bound Au atom triggered by CO adsorption. Physical Review B, 2009, 79, .	1.1	6
95	Adsorption of metal adatoms on FeO(111) and MgO(111) monolayers: Effects of charge state of adsorbate on rumpling of supported oxide film. Physical Review B, 2009, 80, .	1.1	49
96	Modifying the Adsorption Characteristic of Inert Silica Films by Inserting Anchoring Sites. Physical Review Letters, 2009, 102, 016102.	2.9	21
97	Realization of an atomic sieve: Silica on Mo(112). Surface Science, 2009, 603, 1145-1149.	0.8	25
98	X-ray Photoemission Study of the Charge State of Au Nanoparticles on Thin MgO/Fe(001) Films. Journal of Physical Chemistry C, 2009, 113, 19957-19965.	1.5	27
99	Tailoring the Interaction Strength between Gold Particles and Silica Thin Films via Work Function Control. Physical Review Letters, 2009, 103, 056801.	2.9	37
100	Adsorption of Late Transition Metal Atoms on MgO/Mo(100) and MgO/Ag(100) Ultrathin Films: A Comparative DFT Study. Journal of Physical Chemistry C, 2009, 113, 16694-16701.	1.5	37
101	Lithium incorporation into a silica thin film: Scanning tunneling microscopy and density functional theory. Physical Review B, 2009, 80, .	1.1	21
102	CO Adsorption on One-, Two-, and Three-Dimensional Au Clusters Supported on MgO/Ag(001) Ultrathin Films. Journal of Physical Chemistry C, 2009, 113, 10256-10263.	1.5	29
103	Adsorption of transition metal atoms on the NiO(100) surface and on NiO/Ag(100) thin films. Theoretical Chemistry Accounts, 2008, 120, 575-582.	0.5	15
104	Evidence for a Size-Selective Adsorption Mechanism on Oxide Surfaces: Pd and Au atoms on SiO <sub>2</sub> /Mo(112). ChemPhysChem, 2008, 9, 1367-1370.	1.0	31
105	F and F <sup>+</sup> Centers on MgO/Ag(100) or MgO/Mo(100) Ultrathin Films: Are They Stable?. Journal of Physical Chemistry C, 2008, 112, 3857-3865.	1.5	31
106	Au Dimers on Thin MgO(001) Films: Flat and Charged or Upright and Neutral?. Journal of the American Chemical Society, 2008, 130, 7814-7815.	6.6	62
107	Charge-induced formation of linear Au clusters on thin MgO films: Scanning tunneling microscopy and density-functional theory study. Physical Review B, 2008, 78, .	1.1	64
108	Gold Nanostructures on TiOx/Mo(112) Thin Films. Journal of Physical Chemistry C, 2008, 112, 191-200.	1.5	15

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109	Adsorption of Au and Pd Atoms on Thin SiO <sub>2</sub> Films: the Role of Atomic Structure. Journal of Physical Chemistry C, 2008, 112, 3405-3409.	1.5	29
110	Tuning the work function of ultrathin oxide films on metals by adsorption of alkali atoms. Journal of Chemical Physics, 2008, 128, 164707.	1.2	44
111	Charging of Metal Adatoms on Ultrathin Oxide Films: Au and Pd on $\text{FeO}/\text{Pt}$ film. Physical Review B, 2007, 76, .	2.9	109
112	Observable consequences of formation of Au anions from deposition of Au atoms on ultrathin oxide films. Journal of Chemical Physics, 2007, 127, 144713.	1.2	29
113	Interplay between structural, magnetic, and electronic properties in $\text{Fe}/\text{O}/\text{Pt}$ film. Physical Review B, 2007, 76, .	1.1	129
114	Local zero-bias anomaly in tunneling spectra of a transition-metal oxide thin film. Physical Review B, 2007, 75, .	1.1	20
115	Prediction of Uncompensated Polarity in Ultrathin Films. Physical Review Letters, 2007, 98, 205701.	2.9	94
116	Cationic and anionic vacancies on the NiO(100) surface: DFT+U and hybrid functional density functional theory calculations. Journal of Chemical Physics, 2007, 127, 174711.	1.2	93
117	Structure, Composition, and Electronic Properties of TiO <sub>x</sub> /Mo(112) Thin Films. Journal of Physical Chemistry C, 2007, 111, 7437-7445.	1.5	11
118	Electron Trapping at Point Defects on Hydroxylated Silica Surfaces. Physical Review Letters, 2007, 99, 136801.	2.9	45
119	Control of the Charge State of Metal Atoms on Thin MgO Films. Physical Review Letters, 2007, 98, 096107.	2.9	310
120	Optical and EPR properties of point defects at a crystalline silica surface: Ab initio embedded-cluster calculations. Physical Review B, 2007, 75, .	1.1	49
121	Palladium Monomers, Dimers, and Trimers on the MgO(001) Surface Viewed Individually. Angewandte Chemie - International Edition, 2007, 46, 8703-8706.	7.2	32
122	Comment on "The structure of monolayer SiO <sub>2</sub> on Mo(112): A 2-D [Si-O-Si] network or isolated [SiO <sub>4</sub> ] units?" Surface Science, 2007, 601, 588-590.	0.8	10
123	The structure of a stoichiometric TiO <sub>2</sub> nanophase on Pt(1 1 1). Surface Science, 2007, 601, 3488-3496.	0.8	40
124	Theory of oxides surfaces, interfaces and supported nano-clusters. Theoretical Chemistry Accounts, 2007, 117, 827-845.	0.5	30
125	Nature of Point Defects on SiO <sub>2</sub> /Mo(112) Thin Films and Their Interaction with Au Atoms. Journal of Physical Chemistry B, 2006, 110, 17015-17023.	1.2	28
126	Charge transfers at metal/oxide interfaces: a DFT study of formation of K <sup>+</sup> and Au <sup>+</sup> species on MgO/Ag(100) ultra-thin films from deposition of neutral atoms. Physical Chemistry Chemical Physics, 2006, 8, 3335-3341.	1.3	82



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127	Vibrational and electron paramagnetic resonance properties of free and MgO supported AuCO complexes. <i>Journal of Chemical Physics</i> , 2006, 124, 174709.	1.2	25
128	Nucleation and growth on defect sites: experimentâ€“theory comparison for Pd/MgO(001). <i>Journal of Physics Condensed Matter</i> , 2006, 18, S411-S427.	0.7	26
129	Au and Pd atoms adsorbed on pure and Ti-doped SiO <sub>2</sub> •Mo(112) films. <i>Journal of Chemical Physics</i> , 2006, 124, 034701.	1.2	41
130	Electronic structure of NiOâ€“Ag(100) thin films from DFT+U and hybrid functional DFT approaches. <i>Physical Review B</i> , 2006, 74, .	1.1	68
131	When the Reporter Induces the Effect: Unusual IR spectra of CO on Au <sub>1</sub> /MgO(001)/Mo(001). <i>Angewandte Chemie - International Edition</i> , 2006, 45, 2633-2635.	7.2	101
132	Tuning the surface metal work function by deposition of ultrathin oxide films: Density functional calculations. <i>Physical Review B</i> , 2006, 73, .	1.1	231
133	CO adsorption on Ni <sub>4</sub> and Ni <sub>8</sub> clusters deposited on regular and defect sites of the MgO(001) surface. <i>Surface Science</i> , 2005, 575, 103-114.	0.8	18
134	Pd nanoclusters at the MgO(100) surface. <i>Surface Science</i> , 2005, 575, 197-209.	0.8	40
135	Structure and vibrational spectra of crystalline SiO <sub>2</sub> ultra-thin films on Mo(112). <i>Surface Science</i> , 2005, 584, 225-236.	0.8	65
136	Formation of Pd dimers at regular and defect sites of the MgO(100) surface: cluster model calculations. <i>Chemical Physics</i> , 2005, 309, 41-47.	0.9	25
137	Charging of Metal Atoms on Ultrathin MgO/Mo(100) Films. <i>Physical Review Letters</i> , 2005, 94, 226104.	2.9	338
138	Acetylene trimerization on Ag, Pd and Rh atoms deposited on MgO thin films. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 955-962.	1.3	42
139	Cluster and Periodic DFT Calculations of MgO/Pd(CO) and MgO/Pd(CO) <sub>2</sub> Surface Complexes. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3416-3422.	1.2	16
140	Bonding of Pd, Ag, and Au atoms on MgO(100) surfaces and MgO•Mo(100) ultra-thin films: A comparative DFT study. <i>Physical Review B</i> , 2005, 72, .	1.1	82
141	Nucleation of Pd Dimers at Defect Sites of the MgO(100) Surface. <i>Physical Review Letters</i> , 2004, 92, 096105.	2.9	101
142	Using Polarity for Engineering Oxide Nanostructures: Structural Phase Diagram in Free and Supported MgO(111) Ultrathin Films. <i>Physical Review Letters</i> , 2004, 93, 215702.	2.9	104
143	Chemistry on single atoms: key factors for the acetylene trimerization on MgO-supported Rh, Pd, and Ag atoms. <i>Chemical Physics Letters</i> , 2004, 399, 266-270.	1.2	29
144	Theoretical evidence for fast H-divacancy rotation on H/Pd(111). <i>Chemical Physics Letters</i> , 2004, 400, 163-168.	1.2	3

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145	Electronic properties of rutileTiO <sub>2</sub> ultrathin films: Odd-even oscillations with the number of layers. Physical Review B, 2004, 70, .	1.1	144
146	Nucleation and growth of Ni clusters on regular sites and F centers on the MgO() surface. Surface Science, 2003, 522, 175-184.	0.8	30
147	CO adsorption on Rh, Pd and Ag atoms deposited on the MgO surface: a comparative ab initio study. Surface Science, 2003, 540, 63-75.	0.8	47
148	Acetylene polymerization on supported transition metal clusters. Journal of Molecular Catalysis A, 2003, 199, 103-113.	4.8	39
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