

M VerÃ³nica Ganduglia-Pirovano

List of Publications by Year in descending order

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108
papers

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57719

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times ranked

7522
citing authors

#	ARTICLE	IF	CITATIONS
1	Oxygen vacancies in transition metal and rare earth oxides: Current state of understanding and remaining challenges. <i>Surface Science Reports</i> , 2007, 62, 219-270.	3.8	1,102
2	Hybrid functionals applied to rare-earth oxides: The example of ceria. <i>Physical Review B</i> , 2007, 75, .	1.1	502
3	Density-Functional Calculations of the Structure of Near-Surface Oxygen Vacancies and Electron Localization on CeO_2 (111) Surfaces. <i>Physical Review Letters</i> , 2013, 110, 246101.	2.9	501
4	Raman Spectra of Polycrystalline CeO_2 : A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 20834-20849.	1.5	278
5	Dry Reforming of Methane on a Highly Active Ni/CeO ₂ Catalyst: Effects of Metal-Support Interactions on C-H Bond Breaking. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 7455-7459.	7.2	276
6	In Situ and Theoretical Studies for the Dissociation of Water on an Active Ni/CeO ₂ Catalyst: Importance of Strong Metal-Support Interactions for the Cleavage of O-H Bonds. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 3917-3921.	7.2	205
7	Catalysis and corrosion: the theoretical surface-science context. <i>Surface Science</i> , 2002, 500, 368-394.	0.8	197
8	Role of Ceria in Oxidative Dehydrogenation on Supported Vanadia Catalysts. <i>Journal of the American Chemical Society</i> , 2010, 132, 2345-2349.	6.6	191
9	Electronic and nuclear chemical reactivity. <i>Journal of Chemical Physics</i> , 1994, 101, 8988-8997.	1.2	170
10	Role of Subsurface Oxygen in Oxide Formation at Transition Metal Surfaces. <i>Physical Review Letters</i> , 2002, 89, 096103.	2.9	166
11	Surface core-level shifts of clean and oxygen-covered Ru(0001). <i>Physical Review B</i> , 2001, 63, .	1.1	163
12	Electron Localization in Defective Ceria Films: A Study with Scanning-Tunneling Microscopy and Density-Functional Theory. <i>Physical Review Letters</i> , 2011, 106, 246801.	2.9	158
13	Room-Temperature Activation of Methane and Dry Re-forming with CO ₂ on Ni-CeO ₂ (111) Surfaces: Effect of Ce ³⁺ Sites and Metal-Support Interactions on C-H Bond Cleavage. <i>ACS Catalysis</i> , 2016, 6, 8184-8191.	5.5	146
14	Direct Conversion of Methane to Methanol on Ni-Ceria Surfaces: Metal-Support Interactions and Water-Enabled Catalytic Conversion by Site Blocking. <i>Journal of the American Chemical Society</i> , 2018, 140, 7681-7687.	6.6	141
15	Resolving the Atomic Structure of Vanadia Monolayer Catalysts: Monomers, Trimers, and Oligomers on Ceria. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 8006-8009.	7.2	138
16	Structural and electronic properties of chemisorbed oxygen on Rh(111). <i>Physical Review B</i> , 1999, 59, 15533-15543.	1.1	127
17	Evidence for Subsurface Ordering of Oxygen Vacancies on the Reduced CeO_2 (111) Surface. <i>Physical Review Letters</i> , 2013, 110, 246101.	2.9	121
18	Atomistic description of oxide formation on metal surfaces: the example of ruthenium. <i>Chemical Physics Letters</i> , 2002, 352, 311-317.	1.2	120

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19	In situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metal-Support Interactions and C-H Bond Activation at Low Temperature. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 13041-13046.	7.2	120
20	Metastable precursors during the oxidation of the Ru(0001) surface. <i>Physical Review B</i> , 2002, 65, .	1.1	119
21	Stability of reduced V ₂ O ₅ (001) surfaces. <i>Physical Review B</i> , 2004, 70, .	1.1	119
22	Insight into the Adsorption of Water on the Clean CeO ₂ (111) Surface with van der Waals and Hybrid Density Functionals. <i>Journal of Physical Chemistry C</i> , 2012, 116, 13584-13593.	1.5	116
23	Surface Metal-Insulator Transition on a Vanadium Pentoxide (001) Single Crystal. <i>Physical Review Letters</i> , 2007, 99, 226103.	2.9	113
24	Reactivity kernels, the normal modes of chemical reactivity, and the hardness and softness spectra. <i>Journal of Chemical Physics</i> , 1995, 103, 3543-3551.	1.2	112
25	Molecular-Level Understanding of CeO ₂ as a Catalyst for Partial Alkyne Hydrogenation. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5352-5360.	1.5	112
26	Hydrogen activation, diffusion, and clustering on CeO ₂ (111): A DFT+U study. <i>Journal of Chemical Physics</i> , 2014, 141, 014703.	1.2	109
27	Counting Electrons Transferred through a Thin Alumina Film into Au Chains. <i>Physical Review Letters</i> , 2008, 100, 096802.	2.9	101
28	Theoretical Studies of the Adsorption of CO and C on Ni(111) and Ni/CeO ₂ (111): Evidence of a Strong Metal-Support Interaction. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8241-8250.	1.5	100
29	Nitrogen adsorption on Fe(111), (100), and (110) surfaces. <i>Surface Science</i> , 1999, 422, 8-16.	0.8	97
30	Comment on "Taming multiple valency with density functionals: A case study of defective ceria". <i>Physical Review B</i> , 2005, 72, .	1.1	90
31	Periodic density functional study on structural and vibrational properties of vanadium oxide aggregates. <i>Physical Review B</i> , 2004, 69, .	1.1	76
32	Oxygen-induced Rh _{3d5/2} surface core-level shifts on Rh(111). <i>Physical Review B</i> , 2001, 63, .	1.1	72
33	Ordering of oxygen vacancies and excess charge localization in bulk ceria: A DFT+U study. <i>Physical Review B</i> , 2014, 90, .	1.1	71
34	Formaldehyde Formation on Vanadium Oxide Surfaces V ₂ O ₃ (0001) and V ₂ O ₅ (001): How does the Stable Methoxy Intermediate Form?. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 3695-3698.	7.2	70
35	Formation of the cerium orthovanadate CeVO ₄ : DFT+U study. <i>Physical Review B</i> , 2007, 76, .	1.1	61
36	Periodic Density Functional Theory Study of VO _n Species Supported on the CeO ₂ (111) Surface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7399-7410.	1.5	61

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37	Experimental and Theoretical Study on the Nature of Adsorbed Oxygen Species on Shaped Ceria Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6593-6598.	2.1	60
38	Orbital symmetry, reactivity, and transition metal surface chemistry. <i>Physical Review Letters</i> , 1994, 72, 3222-3225.	2.9	57
39	Potential, core-level, and d-band shifts at transition-metal surfaces. <i>Physical Review B</i> , 1996, 54, 8892-8898.	1.1	55
40	Low temperature adsorption of oxygen on reduced V ₂ O ₃ (0001) surfaces. <i>Surface Science</i> , 2006, 600, 1497-1503.	0.8	55
41	Selectivity in Methanol Oxidation as Studied on Model Systems Involving Vanadium Oxides. <i>Topics in Catalysis</i> , 2008, 50, 106-115.	1.3	53
42	Stability of subsurface oxygen at Rh(111). <i>Physical Review B</i> , 2002, 65, .	1.1	52
43	d-layer core-level shifts of admetal monolayers on transition-metal substrates and their relation to the surface chemical reactivity. <i>Physical Review B</i> , 1996, 53, 10344-10347.	1.1	50
44	The non-innocent role of cerium oxide in heterogeneous catalysis: A theoretical perspective. <i>Catalysis Today</i> , 2015, 253, 20-32.	2.2	50
45	Insights into the Nature of Formate Species in the Decomposition and Reaction of Methanol over Cerium Oxide Surfaces: A Combined Infrared Spectroscopy and Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21452-21464.	1.5	47
46	Partial oxidation of methanol on well-ordered V ₂ O ₅ (001)/Au(111) thin films. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3290.	1.3	44
47	Hydrogen Spillover to Copper Clusters on Hydroxylated $\hat{\Gamma}^3$ -Al ₂ O ₃ . <i>Journal of Physical Chemistry C</i> , 2018, 122, 18445-18455.	1.5	44
48	Oxygen-Vacancy Dynamics and Entanglement with Polaron Hopping at the Reduced CeO_2 . <i>Journal of Physical Chemistry C</i> , 2018, 122, 18445-18455.	1.5	44
49	Vanadium Oxides on Aluminum Oxide Supports. 1. Surface Termination and Reducibility of Vanadia Films on $\hat{\Gamma}^3$ -Al ₂ O ₃ (0001). <i>Journal of Physical Chemistry B</i> , 2005, 109, 23523-23531.	1.2	42
50	Ni Nanoparticles on CeO ₂ (111): Energetics, Electron Transfer, and Structure by Ni Adsorption Calorimetry, Spectroscopies, and Density Functional Theory. <i>ACS Catalysis</i> , 2020, 10, 5101-5114.	5.5	42
51	Surface Stabilizes Ceria in Unexpected Stoichiometry. <i>Journal of Physical Chemistry C</i> , 2017, 121, 6844-6851.	1.5	40
52	Toward an Atomic-Level Understanding of Ceria-Based Catalysts: When Experiment and Theory Go Hand in Hand. <i>Accounts of Chemical Research</i> , 2021, 54, 2884-2893.	7.6	40
53	Crystal Structure and Vibrational Spectra of AlVO ₄ . A DFT Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 394-400.	1.2	39
54	Reaction Pathway for Coke-Free Methane Steam Reforming on a Ni/CeO ₂ Catalyst: Active Sites and the Role of Metal-Support Interactions. <i>ACS Catalysis</i> , 2021, 11, 8327-8337.	5.5	39

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55	Metal-Support Interactions and C1 Chemistry: Transforming Pt-CeO ₂ into a Highly Active and Stable Catalyst for the Conversion of Carbon Dioxide and Methane. ACS Catalysis, 2021, 11, 1613-1623.	5.5	39
56	Unraveling the oxygen vacancy structures at the reduced CeO ₂ surface. Physical Review Materials, 2018, 2, .	0.9	38
57	Nature of the Active Sites on Ni/CeO ₂ Catalysts for Methane Conversions. ACS Catalysis, 2021, 11, 10604-10613.	5.5	37
58	Identification of single-atom active sites in CO oxidation over oxide-supported Au catalysts. Journal of Catalysis, 2020, 383, 264-272.	3.1	36
59	Dry Reforming of Methane on a Highly-Active Ni-CeO ₂ Catalyst: Effects of Metal-Support Interactions on C-H Bond Breaking. Angewandte Chemie, 2016, 128, 7581-7585.	1.6	35
60	The Structure of Oxygen Vacancies in the Near-Surface of Reduced CeO ₂ (111) Under Strain. Frontiers in Chemistry, 2019, 7, 436.	1.8	34
61	Electron correlations in the ground state of silicon. Physical Review B, 1989, 39, 5156-5164.	1.1	32
62	Electronic properties and charge state of gold monomers and chains adsorbed on alumina thin films on NiAl(110). Physical Review B, 2010, 81, .	1.1	32
63	Adlayer Core-Level Shifts of Random Metal Overlayers on Transition-Metal Substrates. Physical Review Letters, 1997, 78, 1807-1810.	2.9	29
64	Controlled selectivity for ethanol steam reforming reaction over doped CeO ₂ surfaces: The role of gallium. Applied Catalysis B: Environmental, 2020, 277, 119103.	10.8	29
65	Vanadium Oxides on Aluminum Oxide Supports. 2. Structure, Vibrational Properties, and Reducibility of V ₂ O ₅ Clusters on γ -Al ₂ O ₃ (0001). Journal of Physical Chemistry B, 2005, 109, 23532-23542.	1.2	27
66	Vanadium Oxides on Aluminum Oxide Supports. 3. Metastable β -Al ₂ O ₃ (001) Compared to γ -Al ₂ O ₃ (0001). Journal of Physical Chemistry C, 2007, 111, 5141-5153.	1.5	27
67	Breaking Simple Scaling Relations through Metal-Oxide Interactions: Understanding Room-Temperature Activation of Methane on M/CeO ₂ (M = Pt, Ni, or Co) Interfaces. Journal of Physical Chemistry Letters, 2020, 11, 9131-9137.	2.1	27
68	Effect of the surface model on the theoretical description of the chemisorption of atomic hydrogen on Cu(). Surface Science, 2003, 522, 185-197.	0.8	26
69	Diffusion Barriers Block Defect Occupation on Reduced CeO ₂ surface. Physical Review Materials, 2018, 2, .	0.9	38
70	Single Ni Sites Supported on CeO ₂ (111) Reveal Cooperative Effects in the Water-Gas Shift Reaction. Journal of Physical Chemistry C, 2019, 123, 7749-7757.	1.5	23
71	Electronic correlations of cubic boron nitride. Physical Review B, 1991, 44, 3526-3536.	1.1	22
72	Vanadia Aggregates on an Ultrathin Aluminum Oxide Film on NiAl(110). Journal of Physical Chemistry C, 2010, 114, 4983-4994.	1.5	20

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73	Reduction of the (001) Surface of $\hat{V}^3\text{-V}_2\text{O}_5$ Compared to $\hat{V}^{\pm}\text{-V}_2\text{O}_5$. Journal of Physical Chemistry B, 2005, 109, 374-380.	1.2	19
74	Methanol Adsorption on $\text{V}_2\text{O}_3(0001)$. Topics in Catalysis, 2011, 54, 669-684.	1.3	18
75	Orbital and dipolar contributions to the hyperfine fields in bulk bcc Fe, hcp Co, and at the Fe/Ag(100) interface: The inclusion of orbital polarization. Physical Review B, 2001, 63, .	1.1	17
76	Vanadia and Water Coadsorption on Tetragonal Zirconia Surfaces. Journal of Physical Chemistry C, 2009, 113, 18191-18203.	1.5	17
77	Reduced $\langle \text{mml:math} \rangle$ xmlns:mml="http://www.w3.org/1998/Math/MathML">< mml:mrow >< mml:msub >< mml:mi >CeO</mml:mi>< mml:mn >2</mml:mn></mml:mrow>< mml:math >3</mml:math>< mml:mi >O</mml:mi>< mml:mn >5</mml:mn></mml:mrow>< mml:math >O</mml:math>< mml:mn >3</mml:mn></mml:mrow></mml:math> ordered phases as bulk terminations: Introducing the structure of $\langle \text{mml:math} \rangle$ xmlns:mml="http://www.w3.org/1998/Math/MathML">< mml:mrow >< mml:msub >< mml:mi >Ce</mml:mi>< mml:mn >3</mml:mn></mml:mrow>< mml:math >O</mml:math>< mml:mn >5</mml:mn></mml:mrow>< mml:math >O</mml:math>< mml:mn >3</mml:mn></mml:mrow></mml:math> materials, 2018, 2, .	1.9	17
78	Nucleation of gold atoms on vanadyl-terminated $\text{V}_2\text{O}_3(0001)$. New Journal of Physics, 2009, 11, 093007.	1.2	16
79	The structure of epitaxial V_2O_3 films and their surfaces: A medium energy ion scattering study. Surface Science, 2012, 606, 1716-1727.	0.8	16
80	Relative Stability of Near-Surface Oxygen Vacancies at the $\text{CeO}_2(111)$ Surface upon Zirconium Doping. Journal of Physical Chemistry C, 2020, 124, 625-638.	1.5	16
81	Ce=O Terminated CeO_2 . Angewandte Chemie - International Edition, 2021, 60, 13835-13839.	7.2	16
82	Do Au Atoms Titrate Ce^{3+} Ions at the $\text{CeO}_2(111)$ Surface?. Journal of Physical Chemistry C, 2016, 120, 927-933.	1.5	14
83	Insight into the mechanism of the water-gas shift reaction over Au/ CeO_2 catalysts using combined <i>operando</i> spectroscopies. Faraday Discussions, 2021, 229, 232-250.	1.6	14
84	Facet-dependent stability of near-surface oxygen vacancies and excess charge localization at CeO_2 surfaces. Journal of Physics Condensed Matter, 2021, 33, 504003.	0.7	14
85	Enhanced Methanol Production over Non-promoted $\text{Cu}^{\text{Mg}}\text{Al}_2\text{O}_3$ Materials with Ex-solved 2 nm Cu Particles: Insights from an Operando Spectroscopic Study. ACS Catalysis, 2022, 12, 3845-3857.	5.5	14
86	Publisher's Note: Hybrid functionals applied to rare-earth oxides: The example of ceria [Phys. Rev. B75, 045121 (2007)]. Physical Review B, 2007, 75, .	1.1	13
87	Vibrational Frequencies of Cerium-Oxide-Bound CO: A Challenge for Conventional DFT Methods. Physical Review Letters, 2020, 125, 256101.	2.9	13
88	Enhanced oxidation activity from modified ceria: MnOx -ceria, CrOx -ceria and Mg doped VOx -ceria. Applied Catalysis B: Environmental, 2016, 197, 313-323.	10.8	12
89	Theoretical Study of the Catalytic Performance of Activated Layered Double Hydroxides in the Cyanoethylation of Alcohols. Journal of Physical Chemistry C, 2019, 123, 8777-8784.	1.5	12
90	Electronic structure of random Ag-Pd and Ag-vacancy overlayers on an fcc Pd(001) substrate. Physical Review B, 1993, 48, 1870-1876.	1.1	11

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91	Oxygen Defects at Reducible Oxide Surfaces: The Example of Ceria and Vanadia. Springer Series in Surface Sciences, 2015, , 149-190.	0.3	10
92	Comment on "Oxygen Vacancy Ordering and Electron Localization in CeO ₂ : Hybrid Functional Study". Journal of Physical Chemistry C, 2017, 121, 21080-21083.	1.5	10
93	In-Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metal-Support Interactions and C-H Bond Activation at Low Temperature. Angewandte Chemie, 2017, 129, 13221-13226.	1.6	9
94	Elucidating the Oxygen Storage-Release Dynamics in Ceria Nanorods by Combined Multi-Wavelength Raman Spectroscopy and DFT. Journal of Physical Chemistry Letters, 2020, 11, 8554-8559.	2.1	9
95	Interference, resonances, and bound states at the Pd(001) and Rh(001) surfaces. Physical Review B, 1994, 50, 11142-11145.	1.1	7
96	First-principles study of hyperfine fields in a Cd impurity in the Fe/Ag(100) interface. Physical Review B, 2001, 64, .	1.1	7
97	Interaction of HCl with a CeO ₂ (111) Layer Supported on Ru(0001): A Theory and Experiment Combined Study. Journal of Physical Chemistry C, 2018, 122, 19584-19592.	1.5	6
98	Tuning Selectivity in the Direct Conversion of Methane to Methanol: Bimetallic Synergistic Effects on the Cleavage of C-H and O-H Bonds over NiCu/CeO ₂ Catalysts. Journal of Physical Chemistry Letters, 2022, 13, 5589-5596.	2.1	6
99	Nonuniform temperature dependence of the reactivity of disordered VO _x /Al ₂ O ₃ (001) surfaces: A density functional theory based Monte Carlo study. Journal of Chemical Physics, 2008, 129, 224710.	1.2	5
100	Imaging of individual adatoms on oxide surfaces by dynamic force microscopy. Physical Review B, 2010, 81, .	1.1	4
101	Editorial: The Role of Non-stoichiometry in the Functional Properties of Oxide Materials. Frontiers in Chemistry, 2019, 7, 547.	1.8	4
102	Ce=O Terminated CeO ₂ . Angewandte Chemie, 2021, 133, 13954-13958.	1.6	3
103	Chemical Reactivity Theory for Physicists; A Work in Progress. Kluwer International Series in Engineering and Computer Science, 1996, , 315-333.	0.2	2
104	The electronic structure of a model bimetallic catalyst: symmetry-resolved density of states at Γ for Cu/Ru(111). Surface Science, 1995, 331-333, 716-722.	0.8	1
105	Overlayer and interface resonances and bound states at Pd/Ag(001) and Ag/Pd(001) surfaces. Surface Science, 1995, 331-333, 691-696.	0.8	1
106	Publisher's Note: Stability of reduced V ₂ O ₅ (001) surfaces [Phys. Rev. B 70, 045422 (2004)]. Physical Review B, 2004, 70, .	1.1	1
107	Adiabatic limit for the time dependent Coulomb problem. Journal of Chemical Physics, 1986, 84, 3324-3326.	1.2	0
108	A density functional theory based Monte Carlo study of the reactivity of disordered VO _x /Al ₂ O ₃ (001) surfaces. , 2009, , .		0