M VerÃ³nica Ganduglia-Pirovano

List of Publications by Year
in descending order

108 papers	8,193 citations	57719 44 h-index	46771 89 g-index
114 all docs	114 docs citations	114 times ranked	7522 citing authors

#	ARTICLE	IF	CITATIONS
1	Enhanced Methanol Production over Non-promoted Cuâ€“MgOâ€“Al₂O₃ Materials with Ex-solved 2 nm Cu Particles: Insights from an Operando Spectroscopic Study. ACS Catalysis, 2022, 12, 3845-3857.	5.5	14
2	Tuning Selectivity in the Direct Conversion of Methane to Methanol: Bimetallic Synergistic Effects on the Cleavage of Câ€“H and Oâ€“H Bonds over NiCu/CeO₂ Catalysts. Journal of Physical Chemistry Letters, 2022, 13, 5589-5596.	2.1	6
3	Insight into the mechanism of the waterâ€“gas shift reaction over Au/CeO₂ catalysts using combined operando spectroscopies. Faraday Discussions, 2021, 229, 232-250.	1.6	14
4	Ce=O Terminated CeO₂. Angewandte Chemie - International Edition, 2021, 60, 13835-13839.	7.2	16
5	Ce=O Terminated CeO 2. Angewandte Chemie, 2021, 133, 13954-13958.	1.6	3
6	Toward an Atomic-Level Understanding of Ceria-Based Catalysts: When Experiment and Theory Go Hand in Hand. Accounts of Chemical Research, 2021, 54, 2884-2893.	7.6	40
7	Reaction Pathway for Coke-Free Methane Steam Reforming on a Ni/CeO₂ Catalyst: Active Sites and the Role of Metalâ€“Support Interactions. ACS Catalysis, 2021, 11, 8327-8337.	5.5	39
8	Nature of the Active Sites on Ni/CeO₂ Catalysts for Methane Conversions. ACS Catalysis, 2021, 11, 10604-10613.	5.5	37
9	Facet-dependent stability of near-surface oxygen vacancies and excess charge localization at CeO₂ surfaces. Journal of Physics Condensed Matter, 2021, 33, 504003.	0.7	14
10	Metalâ€“Support Interactions and C1 Chemistry: Transforming Pt-CeO₂ into a Highly Active and Stable Catalyst for the Conversion of Carbon Dioxide and Methane. ACS Catalysis, 2021, 11, 1613-1623.	5.5	39
11	Relative Stability of Near-Surface Oxygen Vacancies at the CeO₂(111) Surface upon Zirconium Doping. Journal of Physical Chemistry C, 2020, 124, 625-638.	1.5	16
12	Breaking Simple Scaling Relations through Metalâ€“Oxide Interactions: Understanding Room-Temperature Activation of Methane on M/CeO₂ (M = Pt, Ni, or Co) Interfaces. Journal of Physical Chemistry Letters, 2020, 11, 9131-9137.	2.1	27
13	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
14	Controlled selectivity for ethanol steam reforming reaction over doped CeO2 surfaces: The role of gallium. Applied Catalysis B: Environmental, 2020, 277, 119103.	10.8	29
15	Ni Nanoparticles on CeO₂(111): Energetics, Electron Transfer, and Structure by Ni Adsorption Calorimetry, Spectroscopies, and Density Functional Theory. ACS Catalysis, 2020, 10, 5101-5114.	5.5	42
16	Identification of single-atom active sites in CO oxidation over oxide-supported Au catalysts. Journal of Catalysis, 2020, 383, 264-272.	3.1	36
17	Vibrational Frequencies of Cerium-Oxide-Bound CO: A Challenge for Conventional DFT Methods. Physical Review Letters, 2020, 125, 256101.	2.9	13
18	Editorial: The Role of Non-stoichiometry in the Functional Properties of Oxide Materials. Frontiers in Chemistry, 2019, 7, 547.	1.8	4

#	ARTICLE	IF	CITATIONS
19	The Structure of Oxygen Vacancies in the Near-Surface of Reduced CeO2 (111) Under Strain. Frontiers in Chemistry, 2019, 7, 436.	1.8	34
20	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
21	Oxygen Vacancy Dynamics and Entanglement with Polaron Hopping at the Reduced <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CeO</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub> stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 652 Td (stretchy="false	2.9	43
22	096101. Single Ni Sites Supported on CeO₂(111) Reveal Cooperative Effects in the Waterâ€“Gas Shift Reaction. Journal of Physical Chemistry C, 2019, 123, 7749-7757.	1.5	23
23	Experimental and Theoretical Study on the Nature of Adsorbed Oxygen Species on Shaped Ceria Nanoparticles. Journal of Physical Chemistry Letters, 2018, 9, 6593-6598.	2.1	60
24	Direct Conversion of Methane to Methanol on Ni-Ceria Surfaces: Metalâ€“Support Interactions and Water-Enabled Catalytic Conversion by Site Blocking. Journal of the American Chemical Society, 2018, 140, 7681-7687.	6.6	141
25	Hydrogen Spillover to Copper Clusters on Hydroxylated Î³-Al₂O₃. Journal of Physical Chemistry C, 2018, 122, 18445-18455.	1.5	44
26	Interaction of HCl with a CeO₂(111) Layer Supported on Ru(0001): A Theory and Experiment Combined Study. Journal of Physical Chemistry C, 2018, 122, 19584-19592.	1.5	6
27	Unraveling the oxygen vacancy structures at the reduced <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ce</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>111</mml:mn>	0.9	38
28	Reduced <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CeO</mml:mi><mml:mn>2</mml:mn></mml:msub> ordered phases as bulk terminations: Introducing the structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ce</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml: mathvariant="normal">O</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:. Physical Review Materials, 2018, 2, .	0.9	17
29	Surface Stabilizes Ceria in Unexpected Stoichiometry. Journal of Physical Chemistry C, 2017, 121, 6844-6851.	1.5	40
30	Raman Spectra of Polycrystalline CeO₂: A Density Functional Theory Study. Journal of Physical Chemistry C, 2017, 121, 20834-20849.	1.5	278
31	Comment on â€œOxygen Vacancy Ordering and Electron Localization in CeO₂: Hybrid Functional Studyâ€. Journal of Physical Chemistry C, 2017, 121, 21080-21083.	1.5	10
32	Inâ€…Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metalâ€“Support Interactions and Câ^'H Bond Activation at Low Temperature. Angewandte Chemie, 2017, 129, 13221-13226.	1.6	9
33	Inâ€…Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metalâ€“Support Interactions and Câ^'H Bond Activation at Low Temperature. Angewandte Chemie - International Edition, 2017, 56, 13041-13046.	7.2	120
34	Dry Reforming of Methane on a Highlyâ€Active Niâ€CeO₂ Catalyst: Effects of Metalâ€Support Interactions on Câ^'H Bond Breaking. Angewandte Chemie - International Edition, 2016, 55, 7455-7459.	7.2	276
35	Dry Reforming of Methane on a Highlyâ€Active Niâ€CeO₂ Catalyst: Effects of Metalâ€Support Interactions on Câ^'H Bond Breaking. Angewandte Chemie, 2016, 128, 7581-7585.	1.6	35
36	Diffusion Barriers Block Defect Occupation on Reduced<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CeO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:m stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 47 Td (stretchy="false">)</mml	2.9	25

#	ARTICLE	IF	CITATIONS
37	Room-Temperature Activation of Methane and Dry Re-forming with CO₂ on Ni-CeO₂(111) Surfaces: Effect of Ce³⁺ Sites and Metalâ€“Support Interactions on Câ€“H Bond Cleavage. ACS Catalysis, 2016, 6, 8184-8191.	5.5	146
38	Enhanced oxidation activity from modified ceria: MnOxâ€“ceria, CrOxâ€“ceria and Mg doped VOxâ€“ceria. Applied Catalysis B: Environmental, 2016, 197, 313-323.	10.8	12
39	Do Au Atoms Titrate Ce³⁺ Ions at the CeO_{2â€“x}(111) Surface?. Journal of Physical Chemistry C, 2016, 120, 927-933.	1.5	14
40	In Situ and Theoretical Studies for the Dissociation of Water on an Active Ni/CeO₂ Catalyst: Importance of Strong Metalâ€“Support Interactions for the Cleavage of Oâ€“H Bonds. Angewandte Chemie - International Edition, 2015, 54, 3917-3921.	7.2	205
41	Oxygen Defects at Reducible Oxide Surfaces: The Example of Ceria and Vanadia. Springer Series in Surface Sciences, 2015, , 149-190.	0.3	10
42	The non-innocent role of cerium oxide in heterogeneous catalysis: A theoretical perspective. Catalysis Today, 2015, 253, 20-32.	2.2	50
43	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. Journal of Physical Chemistry C, 2015, 119, 21452-21464.	1.5	47
44	Hydrogen activation, diffusion, and clustering on CeO2(111): A DFT+U study. Journal of Chemical Physics, 2014, 141, 014703.	1.2	109
45	Ordering of oxygen vacancies and excess charge localization in bulk ceria: A<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>study. Physical Review B, 2014, 90, .	1.1	71
46	Molecular-Level Understanding of CeO₂ as a Catalyst for Partial Alkyne Hydrogenation. Journal of Physical Chemistry C, 2014, 118, 5352-5360.	1.5	112
47	Theoretical Studies of the Adsorption of CO and C on Ni(111) and Ni/CeO₂(111): Evidence of a Strong Metalâ€“Support Interaction. Journal of Physical Chemistry C, 2013, 117, 8241-8250.	1.5	100
48	Evidence for Subsurface Ordering of Oxygen Vacancies on the Reduced<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CeO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 292 Td (stretchy="false">)</mm	2.9	121
49	Calculations. Physical Review Letters, 2013, 110, 246101. Insight into the Adsorption of Water on the Clean CeO₂(111) Surface with van der Waals and Hybrid Density Functionals. Journal of Physical Chemistry C, 2012, 116, 13584-13593.	1.5	116
50	The structure of epitaxial V2O3 films and their surfaces: A medium energy ion scattering study. Surface Science, 2012, 606, 1716-1727.	0.8	16
51	Periodic Density Functional Theory Study of VO_n Species Supported on the CeO₂(111) Surface. Journal of Physical Chemistry C, 2011, 115, 7399-7410.	1.5	61
52	Electron Localization in Defective Ceria Films: A Study with Scanning-Tunneling Microscopy and Density-Functional Theory. Physical Review Letters, 2011, 106, 246801.	2.9	158
53	Methanol Adsorption on V2O3(0001). Topics in Catalysis, 2011, 54, 669-684.	1.3	18
54	Imaging of individual adatoms on oxide surfaces by dynamic force microscopy. Physical Review B, 2010, 81, .	1.1	4

#	ARTICLE	IF	CITATIONS
55	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
56	Role of Ceria in Oxidative Dehydrogenation on Supported Vanadia Catalysts. Journal of the American Chemical Society, 2010, 132, 2345-2349.	6.6	191
57	Vanadia Aggregates on an Ultrathin Aluminum Oxide Film on NiAl(110). Journal of Physical Chemistry C, 2010, 114, 4983-4994.	1.5	20
58	A density functional theory based Monte Carlo study of the reactivity of disordered VO[sub x]â^•Î²-Al[sub 2]O[sub 3] (001) surfaces. , 2009, , .		0
59	Density-Functional Calculations of the Structure of Near-Surface Oxygen Vacancies and Electron Localization on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CeO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 567 Td (stretchy="fals	2.9	501
60	Nucleation of gold atoms on vanadyl-terminated V₂O₃(0001). New Journal of Physics, 2009, 11, 093007.	1.2	16
61	Formaldehyde Formation on Vanadium Oxide Surfaces V₂O₃(0001) and V₂O₅(001): How does the Stable Methoxy Intermediate Form?. Angewandte Chemie - International Edition, 2009, 48, 3695-3698.	7.2	70
62	Resolving the Atomic Structure of Vanadia Monolayer Catalysts: Monomers, Trimers, and Oligomers on Ceria. Angewandte Chemie - International Edition, 2009, 48, 8006-8009.	7.2	138
63	Vanadia and Water Coadsorption on Tetragonal Zirconia Surfaces. Journal of Physical Chemistry C, 2009, 113, 18191-18203.	1.5	17
64	Partial oxidation of methanol on well-ordered V2O5(001)/Au(111) thin films. Physical Chemistry Chemical Physics, 2009, 11, 3290.	1.3	44
65	Selectivity in Methanol Oxidation as Studied on Model Systems Involving Vanadium Oxides. Topics in Catalysis, 2008, 50, 106-115.	1.3	53
66	Counting Electrons Transferred through a Thin Alumina Film into Au Chains. Physical Review Letters, 2008, 100, 096802.	2.9	101
67	Nonuniform temperature dependence of the reactivity of disordered VOx/Î²-Al2O3(001) surfaces: A density functional theory based Monte Carlo study. Journal of Chemical Physics, 2008, 129, 224710.	1.2	5
68	Surface Metal-Insulator Transition on a Vanadium Pentoxide (001) Single Crystal. Physical Review Letters, 2007, 99, 226103.	2.9	113
69	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
70	Hybrid functionals applied to rare-earth oxides: The example of ceria. Physical Review B, 2007, 75, .	1.1	502
71	Vanadium Oxides on Aluminum Oxide Supports. 3. Metastable Î²-Al2O3(001) Compared to Î±-Al2O3(0001). Journal of Physical Chemistry C, 2007, 111, 5141-5153.	1.5	27
72	Oxygen vacancies in transition metal and rare earth oxides: Current state of understanding and remaining challenges. Surface Science Reports, 2007, 62, 219-270.	3.8	1,102

#	Article	IF	Citations
73	Formation of the cerium orthovanadateCeVO4:DFT+Ustudy. Physical Review B, 2007, 76, .	1.1	61
74	Low temperature adsorption of oxygen on reduced V2O3(0001) surfaces. Surface Science, 2006, 600, 1497-1503.	0.8	55
75	Comment on â€œTaming multiple valency with density functionals: A case study of defective ceriaâ€. Physical Review B, 2005, 72, .	1.1	90
76	Reduction of the (001) Surface of Î³-V2O5Compared to Î±-V2O5. Journal of Physical Chemistry B, 2005, 109, 374-380.	1.2	19
77	Vanadium Oxides on Aluminum Oxide Supports. 2. Structure, Vibrational Properties, and Reducibility of V2O5 Clusters on Î±-Al2O3(0001). Journal of Physical Chemistry B, 2005, 109, 23532-23542.	1.2	27
78	Vanadium Oxides on Aluminum Oxide Supports. 1. Surface Termination and Reducibility of Vanadia Films on Î±-Al2O3(0001). Journal of Physical Chemistry B, 2005, 109, 23523-23531.	1.2	42
79	Crystal Structure and Vibrational Spectra of AlVO4. A DFT Study. Journal of Physical Chemistry B, 2005, 109, 394-400.	1.2	39
80	Stability of reducedV2O5(001)surfaces. Physical Review B, 2004, 70, .	1.1	119
81	Publisher's Note: Stability of reducedV2O5(001)surfaces [Phys. Rev. B70, 045422 (2004)]. Physical Review B, 2004, 70, .	1.1	1
82	Periodic density functional study on structural and vibrational properties of vanadium oxide aggregates. Physical Review B, 2004, 69, .	1.1	76
83	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
84	Role of Subsurface Oxygen in Oxide Formation at Transition Metal Surfaces. Physical Review Letters, 2002, 89, 096103.	2.9	166
85	Stability of subsurface oxygen at Rh(111). Physical Review B, 2002, 65, .	1.1	52
86	Metastable precursors during the oxidation of the Ru(0001) surface. Physical Review B, 2002, 65, .	1.1	119
87	Catalysis and corrosion: the theoretical surface-science context. Surface Science, 2002, 500, 368-394.	0.8	197
88	Atomistic description of oxide formation on metal surfaces: the example of ruthenium. Chemical Physics Letters, 2002, 352, 311-317.	1.2	120
89	First-principles study of hyperfine fields in a Cd impurity in the Fe/Ag(100) interface. Physical Review B, 2001, 64, .	1.1	7
90	Surface core-level shifts of clean and oxygen-covered Ru(0001). Physical Review B, 2001, 63, .	1.1	163

#	Article	IF	Citations
91	Oxygen-induced Rh3d5/2surface core-level shifts on Rh(111). Physical Review B, 2001, 63, .	1.1	72
92	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
93	Structural and electronic properties of chemisorbed oxygen on Rh(111). Physical Review B, 1999, 59, 15533-15543.	1.1	127
94	Nitrogen adsorption on Fe(111), (100), and (110) surfaces. Surface Science, 1999, 422, 8-16.	0.8	97
95	Adlayer Core-Level Shifts of Random Metal Overlayers on Transition-Metal Substrates. Physical Review Letters, 1997, 78, 1807-1810.	2.9	29
96	Adlayer core-level shifts of admetal monolayers on transition-metal substrates and their relation to the surface chemical reactivity. Physical Review B, 1996, 53, 10344-10347.	1.1	50
97	Potential, core-level, anddband shifts at transition-metal surfaces. Physical Review B, 1996, 54, 8892-8898.	1.1	55
98	Chemical Reactivity Theory for Physicists; A Work in Progress. Kluwer International Series in Engineering and Computer Science, 1996, , 315-333.	0.2	2
99	The electronic structure of a model bimetallic catalyst: symmetry-resolved density of states at Î“Ì…gG for Cu/Ru(111). Surface Science, 1995, 331-333, 716-722.	0.8	1
100	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
101	Reactivity kernels, the normal modes of chemical reactivity, and the hardness and softness spectra. Journal of Chemical Physics, 1995, 103, 3543-3551.	1.2	112
102	Electronic and nuclear chemical reactivity. Journal of Chemical Physics, 1994, 101, 8988-8997.	1.2	170
103	Interference, resonances, and bound states at the Pd(001) and Rh(001) surfaces. Physical Review B, 1994, 50, 11142-11145.	1.1	7
104	Orbital symmetry, reactivity, and transition metal surface chemistry. Physical Review Letters, 1994, 72, 3222-3225.	2.9	57
105	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
106	Electronic correlations of cubic boron nitride. Physical Review B, 1991, 44, 3526-3536.	1.1	22
107	Electron correlations in the ground state of silicon. Physical Review B, 1989, 39, 5156-5164.	1.1	32
108	Adiabatic limit for the time dependent Coulomb problem. Journal of Chemical Physics, 1986, 84, 3324-3326.	1.2	0