Aleksandra Vojvodic

List of Publications by Year
in descending order

80 papers	15,812 citations	57631 44 h-index	62479 80 g-index
86 all docs	86 docs citations	86 times ranked	17246 citing authors

#	Article	IF	Citations
1	Homogeneously dispersed multimetal oxygen-evolving catalysts. Science, 2016, 352, 333-337.	6.0	1,948
2	A highly active and stable IrO _x /SrIrO ₃ catalyst for the oxygen evolution reaction. Science, 2016, 353, 1011-1014.	6.0	1,606
3	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. Journal of Catalysis, 2015, 328, 36-42.	3.1	1,271
4	Materials for solar fuels and chemicals. Nature Materials, 2017, 16, 70-81.	13.3	1,163
5	Two-Dimensional Molybdenum Carbide (MXene) as an Efficient Electrocatalyst for Hydrogen Evolution. ACS Energy Letters, 2016, 1, 589-594.	8.8	1,100
6	Theoretical Investigation of the Activity of Cobalt Oxides for the Electrochemical Oxidation of Water. Journal of the American Chemical Society, 2013, 135, 13521-13530.	6.6	1,093
7	The Challenge of Electrochemical Ammonia Synthesis: A New Perspective on the Role of Nitrogen Scaling Relations. ChemSusChem, 2015, 8, 2180-2186.	3.6	1,018
8	Gold-supported cerium-doped NiOx catalysts for water oxidation. Nature Energy, 2016, 1, .	19.8	458
9	Effects of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>-band shape on the surface reactivity of transition-metal alloys. Physical Review B, 2014, 89, .	1.1	387
10	Exploring the limits: A low-pressure, low-temperature Haberâ€“Bosch process. Chemical Physics Letters, 2014, 598, 108-112.	1.2	369
11	Optimizing Perovskites for the Water-Splitting Reaction. Science, 2011, 334, 1355-1356.	6.0	349
12	Assessing the reliability of calculated catalytic ammonia synthesis rates. Science, 2014, 345, 197-200.	6.0	319
13	Using natureâ€™s blueprint to expand catalysis with Earth-abundant metals. Science, 2020, 369, .	6.0	306
14	Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides. Journal of Physical Chemistry C, 2012, 116, 21077-21082.	1.5	305
15	Tuning the Basal Plane Functionalization of Two-Dimensional Metal Carbides (MXenes) To Control Hydrogen Evolution Activity. ACS Applied Energy Materials, 2018, 1, 173-180.	2.5	304
16	New design paradigm for heterogeneous catalysts. National Science Review, 2015, 2, 140-143.	4.6	280
17	Electronic Structure Effects in Transition Metal Surface Chemistry. Topics in Catalysis, 2014, 57, 25-32.	1.3	238
18	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. Physical Chemistry Chemical Physics, 2012, 14, 49-70.	1.3	198

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19	Enhancing Catalytic CO Oxidation over Co₃O₄ Nanowires by Substituting Co²⁺ with Cu²⁺. ACS Catalysis, 2015, 5, 4485-4491.	5.5	183
20	2H-MoS₂ on Mo₂CT_x MXene Nanohybrid for Efficient and Durable Electrocatalytic Hydrogen Evolution. ACS Nano, 2020, 14, 16140-16155.	7.3	180
21	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO₂(110) by Transitionâ€Metal Substitution. ChemCatChem, 2011, 3, 1607-1611.	1.8	169
22	Bioinspiration in light harvesting and catalysis. Nature Reviews Materials, 2020, 5, 828-846.	23.3	136
23	On the behavior of BrÃ¸nsted-Evans-Polanyi relations for transition metal oxides. Journal of Chemical Physics, 2011, 134, 244509.	1.2	128
24	Edge reactivity and water-assisted dissociation on cobalt oxide nanoislands. Nature Communications, 2017, 8, 14169.	5.8	117
25	MXene Materials for the Electrochemical Nitrogen Reductionâ€"Functionalized or Not?. ACS Catalysis, 2020, 10, 253-264.	5.5	107
26	Improving Oxygen Electrochemistry through Nanoscopic Confinement. ChemCatChem, 2015, 7, 738-742.	1.8	106
27	Effects of Applied Potential and Water Intercalation on the Surface Chemistry of Ti₂C and Mo₂C MXenes. Journal of Physical Chemistry C, 2016, 120, 28432-28440.	1.5	104
28	Magnetic edge states in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MoS</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> nanoribbons using density-functional theory. Physical Review B, 2009, 80, .	3.7	97
29	Elementary steps of syngas reactions on Mo2C(001): Adsorption thermochemistry and bond dissociation. Journal of Catalysis, 2012, 290, 108-117.	3.1	96
30	From Electronic Structure to Catalytic Activity: A Single Descriptor for Adsorption and Reactivity on Transition-Metal Carbides. Physical Review Letters, 2009, 103, 146103.	2.9	95
31	Trends in adsorption of electrocatalytic water splitting intermediates on cubic ABO₃ oxides. Physical Chemistry Chemical Physics, 2018, 20, 3813-3818.	1.3	94
32	Electronic Origin of the Surface Reactivity of Transition-Metal-Doped TiO₂(110). Journal of Physical Chemistry C, 2013, 117, 460-465.	1.5	87
33	Activation of ultrathin SrTiO₃ with subsurface SrRuO₃ for the oxygen evolution reaction. Energy and Environmental Science, 2018, 11, 1762-1769.	15.6	83
34	Computational Design of Active Site Structures with Improved Transition-State Scaling for Ammonia Synthesis. ACS Catalysis, 2018, 8, 4017-4024.	5.5	80
35	Interface Controlled Oxidation States in Layered Cobalt Oxide Nanoislands on Gold. ACS Nano, 2015, 9, 2445-2453.	7.3	78
36	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101.	1.2	77

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37	Two-Dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach. Journal of Physical Chemistry Letters, 2015, 6, 1577-1585.	2.1	75
38	BrÃ¸nstedâ€“Evansâ€“Polanyi Relationship for Transition Metal Carbide and Transition Metal Oxide Surfaces. Journal of Physical Chemistry C, 2013, 117, 4168-4171.	1.5	67
39	Water Dissociative Adsorption on NiO(111): Energetics and Structure of the Hydroxylated Surface. ACS Catalysis, 2016, 6, 7377-7384.	5.5	67
40	Influence of Adsorbed Water on the Oxygen Evolution Reaction on Oxides. Journal of Physical Chemistry C, 2015, 119, 1032-1037.	1.5	66
41	Computational Screening of 2D Ordered Double Transition-Metal Carbides (MXenes) as Electrocatalysts for Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2020, 124, 10584-10592.	1.5	62
42	Theoretical evaluation of the surface electrochemistry of perovskites with promising photon absorption properties for solar water splitting. Physical Chemistry Chemical Physics, 2015, 17, 2634-2640.	1.3	58
43	Two-Dimensional Materials as Catalysts for Energy Conversion. Catalysis Letters, 2016, 146, 1917-1921.	1.4	58
44	Binding of polycyclic aromatic hydrocarbons and graphene dimers in density functional theory. New Journal of Physics, 2010, 12, 013017.	1.2	55
45	Theoretical Insights to Bulk Activity Towards Oxygen Evolution in Oxyhydroxides. Catalysis Letters, 2017, 147, 1533-1539.	1.4	43
46	Surface energetics of alkaline-earth metal oxides: Trends in stability and adsorption of small molecules. Physical Review B, 2015, 91, .	1.1	41
47	The Effect of Fe Dopant Location in Co(Fe)OOH_x Nanoparticles for the Oxygen Evolution Reaction. ACS Nano, 2021, 15, 18226-18236.	7.3	37
48	Trends in atomic adsorption on titanium carbide and nitride. Surface Science, 2006, 600, 3619-3623.	0.8	33
49	Trends in bulk electron-structural features of rocksalt early transition-metal carbides. Journal of Physics Condensed Matter, 2010, 22, 375501.	0.7	30
50	An orbital-overlap model for minimal work functions of cesiated metal surfaces. Journal of Physics Condensed Matter, 2012, 24, 445007.	0.7	29
51	Comparative Analysis of Cobalt Oxide Nanoisland Stability and Edge Structures on Three Related Noble Metal Surfaces: Au(111), Pt(111) and Ag(111). Topics in Catalysis, 2017, 60, 503-512.	1.3	29
52	Computationally Probing the Performance of Hybrid, Heterogeneous, and Homogeneous Iridiumâ€Based Catalysts for Water Oxidation. ChemCatChem, 2016, 8, 1792-1798.	1.8	26
53	Steam Reforming on Transition-Metal Carbides from Density-Functional Theory. Catalysis Letters, 2012, 142, 728-735.	1.4	24
54	Atomic and molecular adsorption on transition-metal carbide (111) surfaces from density-functional theory: a trend study of surface electronic factors. Journal of Physics Condensed Matter, 2010, 22, 375504.	0.7	23

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55	Enhancing Oxygen Exchange Activity by Tailoring Perovskite Surfaces. Journal of Physical Chemistry Letters, 2019, 10, 4082-4088.	2.1	23
56	Providing Atomistic Insights into the Dissolution of Rutile Oxides in Electrocatalytic Water Splitting. Journal of Physical Chemistry C, 2022, 126, 922-932.	1.5	22
57	Inherent Enhancement of Electronic Emission from Hexaboride Heterostructure. Physical Review Applied, 2014, 2, .	1.5	20
58	Trends in the Thermodynamic Stability of Ultrathin Supported Oxide Films. Journal of Physical Chemistry C, 2016, 120, 10351-10360.	1.5	19
59	Surface stability of perovskite oxides under OER operating conditions: a first principles approach. Faraday Discussions, 2021, 229, 75-88.	1.6	19
60	Nature of versatile chemisorption on TiC(111) and TiN(111) surfaces. Solid State Communications, 2007, 141, 48-52.	0.9	18
61	TEM and DFT investigation of CVD TiN/Îºâ€“Al2O3 multilayer coatings. Surface and Coatings Technology, 2007, 202, 522-531.	2.2	16
62	Nature of chemisorption on titanium carbide and nitride. Surface Science, 2006, 600, 1612-1618.	0.8	14
63	Structural and electronic properties of Fe dopants in cobalt oxide nanoislands on Au(111). Journal of Chemical Physics, 2019, 150, 041731.	1.2	14
64	DFT Study of Atomically-Modified Alkali-Earth Metal Oxide Films on Tungsten. Journal of Physical Chemistry C, 2014, 118, 11303-11309.	1.5	13
65	Modeling Exsolution of Pt from ATiO₃ Perovskites (A = Ca/Sr/Ba) Using First-Principles Methods. Chemistry of Materials, 2020, 32, 9642-9649.	3.2	11
66	Reviving Inert Oxides for Electrochemical Water Splitting by Subsurface Engineering. Chemistry of Materials, 2020, 32, 5569-5578.	3.2	11
67	Thermionic current densities from first principles. Journal of Chemical Physics, 2013, 138, 204701.	1.2	10
68	Zener tunneling between Wannierâ€“Stark levels in GaAs/AlGaAs superlattices. Solid State Communications, 2005, 136, 580-584.	0.9	7
69	Screened Hybrid Exact Exchange Correction Scheme for Adsorption Energies on Perovskite Oxides. Journal of Physical Chemistry C, 2015, 119, 17662-17666.	1.5	7
70	NGenE 2021: Electrochemistry Is Everywhere. ACS Energy Letters, 2022, 7, 368-374.	8.8	6
71	Stability of Pt-Modified Cu(111) in the Presence of Oxygen and Its Implication on the Overall Electronic Structure. Journal of Physical Chemistry C, 2013, 117, 16371-16380.	1.5	5
72	Anisotropic iron-doping patterns in two-dimensional cobalt oxide nanoislands on Au(111). Nano Research, 2019, 12, 2364-2372.	5.8	4

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73	Role of Undercoordinated Sites for the Catalysis in Confined Spaces Formed by Two-Dimensional Material Overlayers. Journal of Physical Chemistry Letters, 2020, 11, 9400-9407.	2.1	4
74	Improving Oxygen Electrochemistry through Nanoscopic Confinement. ChemCatChem, 2015, 7, 709-709.	1.8	3
75	Coarse-grained model for growth of Î±- and k-Al2O3on TiC and TiN(111): thin alumina films from density-functional calculations. Journal of Physics: Conference Series, 2008, 100, 082010.	0.3	2
76	Computationally Probing the Performance of Hybrid, Heterogeneous, and Homogeneous Iridium-Based Catalysts for Water Oxidation. ChemCatChem, 2016, 8, 1750-1750.	1.8	1
77	Chemistry and Catalysis of MXenes. , 2019, , 445-456.		1
78	Energy Trends in Adsorption at Surfaces. , 2020, , 1321-1341.		1
79	Energy Trends in Adsorption at Surfaces. , 2018, , 1-20.		0
80	Theory: general discussion. Faraday Discussions, 2021, 229, 131-160.	1.6	0