Aleksandra Vojvodic

List of Publications by Citations

79 papers	11,120 citations	42 h-index	86 g-index
86 ext. papers	13,542 ext. citations	10 avg, IF	6.51 L-index

#	Paper	IF	Citations
79	Homogeneously dispersed multimetal oxygen-evolving catalysts. *Science*, **2016**, 352, 333-7	33.3	1459
78	A highly active and stable IrOx/SrIrO3 catalyst for the oxygen evolution reaction. *Science*, **2016**, 353, 1011-1014	33.3	1094
77	Theoretical investigation of the activity of cobalt oxides for the electrochemical oxidation of water. *Journal of the American Chemical Society*, **2013**, 135, 13521-30	16.4	849
76	Materials for solar fuels and chemicals. *Nature Materials*, **2016**, 16, 70-81	27	846
75	Two-Dimensional Molybdenum Carbide (MXene) as an Efficient Electrocatalyst for Hydrogen Evolution. *ACS Energy Letters*, **2016**, 1, 589-594	20.1	752
74	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. *Journal of Catalysis*, **2015**, 328, 36-42	7.3	715
73	The Challenge of Electrochemical Ammonia Synthesis: A New Perspective on the Role of Nitrogen Scaling Relations. *ChemSusChem*, **2015**, 8, 2180-6	8.3	666
72	Gold-supported cerium-doped NiOx catalysts for water oxidation. *Nature Energy*, **2016**, 1,	62.3	366
71	Chemistry. Optimizing perovskites for the water-splitting reaction. *Science*, **2011**, 334, 1355-6	33.3	281
70	Exploring the limits: A low-pressure, low-temperature HaberBosch process. *Chemical Physics Letters*, **2014**, 598, 108-112	2.5	275
69	Catalysis. Assessing the reliability of calculated catalytic ammonia synthesis rates. *Science*, **2014**, 345, 197-200	33.3	244
68	Effects of d-band shape on the surface reactivity of transition-metal alloys. *Physical Review B*, **2014**, 89,	3.3	236
67	Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides. *Journal of Physical Chemistry C*, **2012**, 116, 21077-21082	3.8	236
66	Tuning the Basal Plane Functionalization of Two-Dimensional Metal Carbides (MXenes) To Control Hydrogen Evolution Activity. *ACS Applied Energy Materials*, **2018**, 1, 173-180	6.1	192
65	New design paradigm for heterogeneous catalysts. *National Science Review*, **2015**, 2, 140-143	10.8	191
64	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 49-70	3.6	171
63	Electronic Structure Effects in Transition Metal Surface Chemistry. *Topics in Catalysis*, **2014**, 57, 25-32	2.3	154

62	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO2(110) by Transition-Metal Substitution. *ChemCatChem*, **2011**, 3, 1607-1611	5.2	146
61	Enhancing Catalytic CO Oxidation over Co3O4 Nanowires by Substituting Co2+ with Cu2+. *ACS Catalysis*, **2015**, 5, 4485-4491	13.1	139
60	Using nature's blueprint to expand catalysis with Earth-abundant metals. *Science*, **2020**, 369,	33.3	124
59	On the behavior of Brønsted-Evans-Polanyi relations for transition metal oxides. *Journal of Chemical Physics*, **2011**, 134, 244509	3.9	108
58	Edge reactivity and water-assisted dissociation on cobalt oxide nanoislands. *Nature Communications*, **2017**, 8, 14169	17.4	89
57	Improving Oxygen Electrochemistry through Nanoscopic Confinement. *ChemCatChem*, **2015**, 7, 738-742	5.2	87
56	Magnetic edge states in MoS2 characterized using density-functional theory. *Physical Review B*, **2009**, 80,	3.3	85
55	From electronic structure to catalytic activity: a single descriptor for adsorption and reactivity on transition-metal carbides. *Physical Review Letters*, **2009**, 103, 146103	7.4	85
54	Elementary steps of syngas reactions on Mo2C(001): Adsorption thermochemistry and bond dissociation. *Journal of Catalysis*, **2012**, 290, 108-117	7.3	84
53	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	3.8	80
52	Density functional theory based screening of ternary alkali-transition metal borohydrides: a computational material design project. *Journal of Chemical Physics*, **2009**, 131, 014101	3.9	74
51	Electronic Origin of the Surface Reactivity of Transition-Metal-Doped TiO2(110). *Journal of Physical Chemistry C*, **2013**, 117, 460-465	3.8	72
50	Trends in adsorption of electrocatalytic water splitting intermediates on cubic ABO oxides. *Physical Chemistry Chemical Physics*, **2018**, 20, 3813-3818	3.6	66
49	Interface controlled oxidation states in layered cobalt oxide nanoislands on gold. *ACS Nano*, **2015**, 9, 2445-53	16.7	65
48	2H-MoS on MoCT MXene Nanohybrid for Efficient and Durable Electrocatalytic Hydrogen Evolution. *ACS Nano*, **2020**, 14, 16140-16155	16.7	65
47	Two-Dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach. *Journal of Physical Chemistry Letters*, **2015**, 6, 1577-85	6.4	64
46	MXene Materials for the Electrochemical Nitrogen Reduction□unctionalized or Not?. *ACS Catalysis*, **2020**, 10, 253-264	13.1	60
45	Activation of ultrathin SrTiO3 with subsurface SrRuO3 for the oxygen evolution reaction. *Energy and Environmental Science*, **2018**, 11, 1762-1769	35.4	59

44	Brønsted-Evans-Polanyi Relationship for Transition Metal Carbide and Transition Metal Oxide Surfaces. *Journal of Physical Chemistry C*, **2013**, 117, 4168-4171	3.8	56
43	Influence of Adsorbed Water on the Oxygen Evolution Reaction on Oxides. *Journal of Physical Chemistry C*, **2015**, 119, 1032-1037	3.8	55
42	Bioinspiration in light harvesting and catalysis. *Nature Reviews Materials*, **2020**, 5, 828-846	73.3	54
41	Computational Design of Active Site Structures with Improved Transition-State Scaling for Ammonia Synthesis. *ACS Catalysis*, **2018**, 8, 4017-4024	13.1	52
40	Binding of polycyclic aromatic hydrocarbons and graphene dimers in density functional theory. *New Journal of Physics*, **2010**, 12, 013017	2.9	51
39	Theoretical evaluation of the surface electrochemistry of perovskites with promising photon absorption properties for solar water splitting. *Physical Chemistry Chemical Physics*, **2015**, 17, 2634-40	3.6	49
38	Water Dissociative Adsorption on NiO(111): Energetics and Structure of the Hydroxylated Surface. *ACS Catalysis*, **2016**, 6, 7377-7384	13.1	46
37	Two-Dimensional Materials as Catalysts for Energy Conversion. *Catalysis Letters*, **2016**, 146, 1917-1921	2.8	39
36	Theoretical Insights to Bulk Activity Towards Oxygen Evolution in Oxyhydroxides. *Catalysis Letters*, **2017**, 147, 1533-1539	2.8	35
35	Surface energetics of alkaline-earth metal oxides: Trends in stability and adsorption of small molecules. *Physical Review B*, **2015**, 91,	3.3	34
34	Trends in bulk electron-structural features of rocksalt early transition-metal carbides. *Journal of Physics Condensed Matter*, **2010**, 22, 375501	1.8	30
33	Trends in atomic adsorption on titanium carbide and nitride. *Surface Science*, **2006**, 600, 3619-3623	1.8	30
32	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	3.8	24
31	Steam Reforming on Transition-Metal Carbides from Density-Functional Theory. *Catalysis Letters*, **2012**, 142, 728-735	2.8	22
30	An orbital-overlap model for minimal work functions of cesiated metal surfaces. *Journal of Physics Condensed Matter*, **2012**, 24, 445007	1.8	22
29	Computationally Probing the Performance of Hybrid, Heterogeneous, and Homogeneous Iridium-Based Catalysts for Water Oxidation. *ChemCatChem*, **2016**, 8, 1792-1798	5.2	21
28	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	2.3	19
27	Trends in the Thermodynamic Stability of Ultrathin Supported Oxide Films. *Journal of Physical Chemistry C*, **2016**, 120, 10351-10360	3.8	19

26	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	1.8	18
25	Enhancing Oxygen Exchange Activity by Tailoring Perovskite Surfaces. *Journal of Physical Chemistry Letters*, **2019**, 10, 4082-4088	6.4	17
24	Inherent Enhancement of Electronic Emission from Hexaboride Heterostructure. *Physical Review Applied*, **2014**, 2,	4.3	16
23	Nature of versatile chemisorption on TiC(111) and TiN(111) surfaces. *Solid State Communications*, **2007**, 141, 48-52	1.6	16
22	TEM and DFT investigation of CVD TiN/Al2O3 multilayer coatings. *Surface and Coatings Technology*, **2007**, 202, 522-531	4.4	14
21	Nature of chemisorption on titanium carbide and nitride. *Surface Science*, **2006**, 600, 1612-1618	1.8	13
20	DFT Study of Atomically-Modified Alkali-Earth Metal Oxide Films on Tungsten. *Journal of Physical Chemistry C*, **2014**, 118, 11303-11309	3.8	12
19	Structural and electronic properties of Fe dopants in cobalt oxide nanoislands on Au(111). *Journal of Chemical Physics*, **2019**, 150, 041731	3.9	9
18	Thermionic current densities from first principles. *Journal of Chemical Physics*, **2013**, 138, 204701	3.9	8
17	Reviving Inert Oxides for Electrochemical Water Splitting by Subsurface Engineering. *Chemistry of Materials*, **2020**, 32, 5569-5578	9.6	8
16	Surface stability of perovskite oxides under OER operating conditions: a first principles approach. *Faraday Discussions*, **2021**, 229, 75-88	3.6	8
15	Screened Hybrid Exact Exchange Correction Scheme for Adsorption Energies on Perovskite Oxides. *Journal of Physical Chemistry C*, **2015**, 119, 17662-17666	3.8	7
14	Zener tunneling between Wannier Stark levels in GaAs/AlGaAs superlattices. *Solid State Communications*, **2005**, 136, 580-584	1.6	7
13	The Effect of Fe Dopant Location in Co(Fe)OOH Nanoparticles for the Oxygen Evolution Reaction. *ACS Nano*, **2021**,	16.7	5
12	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	3.8	4
11	Modeling Exsolution of Pt from ATiO3 Perovskites (A = Ca/Sr/Ba) Using First-Principles Methods. *Chemistry of Materials*, **2020**, 32, 9642-9649	9.6	4
10	Providing Atomistic Insights into the Dissolution of Rutile Oxides in Electrocatalytic Water Splitting. *Journal of Physical Chemistry C*, **2022**, 126, 922-932	3.8	3
9	NGenE 2021: Electrochemistry Is Everywhere. *ACS Energy Letters*, **2022**, 7, 368-374	20.1	3

8	Improving Oxygen Electrochemistry through Nanoscopic Confinement. *ChemCatChem*, **2015**, 7, 709-709	5.2	2
7	Coarse-grained model for growth of □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
6	Anisotropic iron-doping patterns in two-dimensional cobalt oxide nanoislands on Au(111). *Nano Research*, **2019**, 12, 2364-2372	10	1
5	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	6.4	0
4	Computationally Probing the Performance of Hybrid, Heterogeneous, and Homogeneous Iridium-Based Catalysts for Water Oxidation. *ChemCatChem*, **2016**, 8, 1750-1750	5.2	0
3	Energy Trends in Adsorption at Surfaces **2020**, 1321-1341		
2	Chemistry and Catalysis of MXenes **2019**, 445-456		
1	Energy Trends in Adsorption at Surfaces **2018**, 1-20		