

# Aleksandra Vojvodic

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Providing Atomistic Insights into the Dissolution of Rutile Oxides in Electrocatalytic Water Splitting. <i>Journal of Physical Chemistry C</i> , <b>2022</b> , 126, 922-932	3.8	3
78	NGenE 2021: Electrochemistry Is Everywhere. <i>ACS Energy Letters</i> , <b>2022</b> , 7, 368-374	20.1	3
77	The Effect of Fe Dopant Location in Co(Fe)OOH Nanoparticles for the Oxygen Evolution Reaction. <i>ACS Nano</i> , <b>2021</b> ,	16.7	5
76	Surface stability of perovskite oxides under OER operating conditions: a first principles approach. <i>Faraday Discussions</i> , <b>2021</b> , 229, 75-88	3.6	8
75	Energy Trends in Adsorption at Surfaces <b>2020</b> , 1321-1341		
74	Reviving Inert Oxides for Electrochemical Water Splitting by Subsurface Engineering. <i>Chemistry of Materials</i> , <b>2020</b> , 32, 5569-5578	9.6	8
73	MXene Materials for the Electrochemical Nitrogen Reduction Functionalized or Not?. <i>ACS Catalysis</i> , <b>2020</b> , 10, 253-264	13.1	60
72	Modeling Exsolution of Pt from ATiO <sub>3</sub> Perovskites (A = Ca/Sr/Ba) Using First-Principles Methods. <i>Chemistry of Materials</i> , <b>2020</b> , 32, 9642-9649	9.6	4
71	2H-MoS <sub>2</sub> on MoCT MXene Nanohybrid for Efficient and Durable Electrocatalytic Hydrogen Evolution. <i>ACS Nano</i> , <b>2020</b> , 14, 16140-16155	16.7	65
70	Bioinspiration in light harvesting and catalysis. <i>Nature Reviews Materials</i> , <b>2020</b> , 5, 828-846	73.3	54
69	Using nature's blueprint to expand catalysis with Earth-abundant metals. <i>Science</i> , <b>2020</b> , 369,	33.3	124
68	Role of Undercoordinated Sites for the Catalysis in Confined Spaces Formed by Two-Dimensional Material Overlayers. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 9400-9407	6.4	0
67	Computational Screening of 2D Ordered Double Transition-Metal Carbides (MXenes) as Electrocatalysts for Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 10584-10592	3.8	24
66	Anisotropic iron-doping patterns in two-dimensional cobalt oxide nanoislands on Au(111). <i>Nano Research</i> , <b>2019</b> , 12, 2364-2372	10	1
65	Enhancing Oxygen Exchange Activity by Tailoring Perovskite Surfaces. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 4082-4088	6.4	17
64	Chemistry and Catalysis of MXenes <b>2019</b> , 445-456		
63	Structural and electronic properties of Fe dopants in cobalt oxide nanoislands on Au(111). <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 041731	3.9	9

62	Activation of ultrathin SrTiO <sub>3</sub> with subsurface SrRuO <sub>3</sub> for the oxygen evolution reaction. <i>Energy and Environmental Science</i> , <b>2018</b> , 11, 1762-1769	35.4	59
61	Trends in adsorption of electrocatalytic water splitting intermediates on cubic ABO oxides. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 3813-3818	3.6	66
60	Tuning the Basal Plane Functionalization of Two-Dimensional Metal Carbides (MXenes) To Control Hydrogen Evolution Activity. <i>ACS Applied Energy Materials</i> , <b>2018</b> , 1, 173-180	6.1	192
59	Computational Design of Active Site Structures with Improved Transition-State Scaling for Ammonia Synthesis. <i>ACS Catalysis</i> , <b>2018</b> , 8, 4017-4024	13.1	52
58	Energy Trends in Adsorption at Surfaces <b>2018</b> , 1-20		
57	Edge reactivity and water-assisted dissociation on cobalt oxide nanoislands. <i>Nature Communications</i> , <b>2017</b> , 8, 14169	17.4	89
56	Theoretical Insights to Bulk Activity Towards Oxygen Evolution in Oxyhydroxides. <i>Catalysis Letters</i> , <b>2017</b> , 147, 1533-1539	2.8	35
55	Comparative Analysis of Cobalt Oxide Nanoisland Stability and Edge Structures on Three Related Noble Metal Surfaces: Au(111), Pt(111) and Ag(111). <i>Topics in Catalysis</i> , <b>2017</b> , 60, 503-512	2.3	19
54	Materials for solar fuels and chemicals. <i>Nature Materials</i> , <b>2016</b> , 16, 70-81	27	846
53	Two-Dimensional Materials as Catalysts for Energy Conversion. <i>Catalysis Letters</i> , <b>2016</b> , 146, 1917-1921	2.8	39
52	A highly active and stable IrO <sub>x</sub> /SrIrO <sub>3</sub> catalyst for the oxygen evolution reaction. <i>Science</i> , <b>2016</b> , 353, 1011-1014	33.3	1094
51	Water Dissociative Adsorption on NiO(111): Energetics and Structure of the Hydroxylated Surface. <i>ACS Catalysis</i> , <b>2016</b> , 6, 7377-7384	13.1	46
50	Gold-supported cerium-doped NiO <sub>x</sub> catalysts for water oxidation. <i>Nature Energy</i> , <b>2016</b> , 1,	62.3	366
49	Computationally Probing the Performance of Hybrid, Heterogeneous, and Homogeneous Iridium-Based Catalysts for Water Oxidation. <i>ChemCatChem</i> , <b>2016</b> , 8, 1792-1798	5.2	21
48	Homogeneously dispersed multimetal oxygen-evolving catalysts. <i>Science</i> , <b>2016</b> , 352, 333-7	33.3	1459
47	Computationally Probing the Performance of Hybrid, Heterogeneous, and Homogeneous Iridium-Based Catalysts for Water Oxidation. <i>ChemCatChem</i> , <b>2016</b> , 8, 1750-1750	5.2	0
46	Effects of Applied Potential and Water Intercalation on the Surface Chemistry of Ti <sub>2</sub> C and Mo <sub>2</sub> C MXenes. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 28432-28440	3.8	80
45	Trends in the Thermodynamic Stability of Ultrathin Supported Oxide Films. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 10351-10360	3.8	19

44	Two-Dimensional Molybdenum Carbide (MXene) as an Efficient Electrocatalyst for Hydrogen Evolution. <i>ACS Energy Letters</i> , <b>2016</b> , 1, 589-594	20.1	752
43	Interface controlled oxidation states in layered cobalt oxide nanoislands on gold. <i>ACS Nano</i> , <b>2015</b> , 9, 2445-53	16.7	65
42	Screened Hybrid Exact Exchange Correction Scheme for Adsorption Energies on Perovskite Oxides. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 17662-17666	3.8	7
41	Enhancing Catalytic CO Oxidation over Co <sub>3</sub> O <sub>4</sub> Nanowires by Substituting Co <sup>2+</sup> with Cu <sup>2+</sup> . <i>ACS Catalysis</i> , <b>2015</b> , 5, 4485-4491	13.1	139
40	Two-Dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 1577-85	6.4	64
39	Influence of Adsorbed Water on the Oxygen Evolution Reaction on Oxides. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 1032-1037	3.8	55
38	Theoretical evaluation of the surface electrochemistry of perovskites with promising photon absorption properties for solar water splitting. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 2634-40	3.6	49
37	Improving Oxygen Electrochemistry through Nanoscopic Confinement. <i>ChemCatChem</i> , <b>2015</b> , 7, 709-709	5.2	2
36	Surface energetics of alkaline-earth metal oxides: Trends in stability and adsorption of small molecules. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	34
35	The Challenge of Electrochemical Ammonia Synthesis: A New Perspective on the Role of Nitrogen Scaling Relations. <i>ChemSusChem</i> , <b>2015</b> , 8, 2180-6	8.3	666
34	New design paradigm for heterogeneous catalysts. <i>National Science Review</i> , <b>2015</b> , 2, 140-143	10.8	191
33	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. <i>Journal of Catalysis</i> , <b>2015</b> , 328, 36-42	7.3	715
32	Improving Oxygen Electrochemistry through Nanoscopic Confinement. <i>ChemCatChem</i> , <b>2015</b> , 7, 738-742	5.2	87
31	Effects of d-band shape on the surface reactivity of transition-metal alloys. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	236
30	Inherent Enhancement of Electronic Emission from Hexaboride Heterostructure. <i>Physical Review Applied</i> , <b>2014</b> , 2,	4.3	16
29	Catalysis. Assessing the reliability of calculated catalytic ammonia synthesis rates. <i>Science</i> , <b>2014</b> , 345, 197-200	33.3	244
28	Electronic Structure Effects in Transition Metal Surface Chemistry. <i>Topics in Catalysis</i> , <b>2014</b> , 57, 25-32	2.3	154
27	DFT Study of Atomically-Modified Alkali-Earth Metal Oxide Films on Tungsten. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 11303-11309	3.8	12

26	Exploring the limits: A low-pressure, low-temperature Haber-Bosch process. <i>Chemical Physics Letters</i> , <b>2014</b> , 598, 108-112	2.5	275
25	Theoretical investigation of the activity of cobalt oxides for the electrochemical oxidation of water. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 13521-30	16.4	849
24	Stability of Pt-Modified Cu(111) in the Presence of Oxygen and Its Implication on the Overall Electronic Structure. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 16371-16380	3.8	4
23	Electronic Origin of the Surface Reactivity of Transition-Metal-Doped TiO <sub>2</sub> (110). <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 460-465	3.8	72
22	Brønsted-Evans-Polanyi Relationship for Transition Metal Carbide and Transition Metal Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 4168-4171	3.8	56
21	Thermionic current densities from first principles. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 204701	3.9	8
20	Elementary steps of syngas reactions on Mo <sub>2</sub> C(001): Adsorption thermochemistry and bond dissociation. <i>Journal of Catalysis</i> , <b>2012</b> , 290, 108-117	7.3	84
19	Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 21077-21082	3.8	236
18	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 49-70	3.6	171
17	Steam Reforming on Transition-Metal Carbides from Density-Functional Theory. <i>Catalysis Letters</i> , <b>2012</b> , 142, 728-735	2.8	22
16	An orbital-overlap model for minimal work functions of cesiated metal surfaces. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 445007	1.8	22
15	Chemistry. Optimizing perovskites for the water-splitting reaction. <i>Science</i> , <b>2011</b> , 334, 1355-6	33.3	281
14	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO <sub>2</sub> (110) by Transition-Metal Substitution. <i>ChemCatChem</i> , <b>2011</b> , 3, 1607-1611	5.2	146
13	On the behavior of Brønsted-Evans-Polanyi relations for transition metal oxides. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 244509	3.9	108
12	Trends in bulk electron-structural features of rocksalt early transition-metal carbides. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 375501	1.8	30
11	Atomic and molecular adsorption on transition-metal carbide (111) surfaces from density-functional theory: a trend study of surface electronic factors. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 375504	1.8	18
10	Binding of polycyclic aromatic hydrocarbons and graphene dimers in density functional theory. <i>New Journal of Physics</i> , <b>2010</b> , 12, 013017	2.9	51
9	Density functional theory based screening of ternary alkali-transition metal borohydrides: a computational material design project. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 014101	3.9	74

8	Magnetic edge states in MoS <sub>2</sub> characterized using density-functional theory. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	85
7	From electronic structure to catalytic activity: a single descriptor for adsorption and reactivity on transition-metal carbides. <i>Physical Review Letters</i> , <b>2009</b> , 103, 146103	7.4	85
6	Coarse-grained model for growth of $\beta$ -Al <sub>2</sub> O <sub>3</sub> on TiC and TiN(111): thin alumina films from density-functional calculations. <i>Journal of Physics: Conference Series</i> , <b>2008</b> , 100, 082010	0.3	2
5	Nature of versatile chemisorption on TiC(111) and TiN(111) surfaces. <i>Solid State Communications</i> , <b>2007</b> , 141, 48-52	1.6	16
4	TEM and DFT investigation of CVD TiN/Al <sub>2</sub> O <sub>3</sub> multilayer coatings. <i>Surface and Coatings Technology</i> , <b>2007</b> , 202, 522-531	4.4	14
3	Nature of chemisorption on titanium carbide and nitride. <i>Surface Science</i> , <b>2006</b> , 600, 1612-1618	1.8	13
2	Trends in atomic adsorption on titanium carbide and nitride. <i>Surface Science</i> , <b>2006</b> , 600, 3619-3623	1.8	30
1	Zener tunneling between Wannier-Stark levels in GaAs/AlGaAs superlattices. <i>Solid State Communications</i> , <b>2005</b> , 136, 580-584	1.6	7