Kai S Exner

List of Publications by Year
in descending order

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56	2,358	218381	214527
papers	citations	26 h-index	47 g-index

57	57	57	1684
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational Pourbaix Diagrams for MXenes: A Key Ingredient toward Proper Theoretical Electrocatalytic Studies. Advanced Theory and Simulations, 2023, 6, .	1.3	16
2	Why the microkinetic modeling of experimental tafel plots requires knowledge of the reaction intermediate's binding energy. Electrochemical Science Advances, 2022, 2, e2100037.	1.2	13
3	Method to Determine the Bifunctional Index for the Oxygen Electrocatalysis from Theory. ChemElectroChem, 2022, 9, .	1.7	13
4	Circumventing the OCl versus OOH scaling relation in the chlorine evolution reaction: Beyond dimensionally stable anodes. Current Opinion in Electrochemistry, 2022, 34, 100979.	2.5	12
5	Statistical analysis of breaking scaling relation in the oxygen evolution reaction. Electrochimica Acta, 2022, 412, 140125.	2.6	12
6	A doxorubicinâ€“peptideâ€“gold nanoparticle conjugate as a functionalized drug delivery system: exploring the limits. Physical Chemistry Chemical Physics, 2022, 24, 14985-14992.	1.3	4
7	On the Optimization of Nitrogenâ€Reduction Electrocatalysts: Breaking Scaling Relation or Catalytic Resonance Theory?. ChemCatChem, 2022, 14, .	1.8	11
8	Computational electrochemistry focusing on nanostructured catalysts: challenges and opportunities. Materials Today Energy, 2022, 28, 101083.	2.5	3
9	Blickpunkt Nachwuchs: Theoretische Elektrokatalyse. Nachrichten Aus Der Chemie, 2022, 70, 82-84.	0.0	0
10	Hydrogen electrocatalysis revisited: Weak bonding of adsorbed hydrogen as the design principle for active electrode materials. Current Opinion in Electrochemistry, 2021, 26, 100673.	2.5	18
11	Boosting the Stability of RuO₂ in the Acidic Oxygen Evolution Reaction by Tuning Oxygenâ€Vacancy Formation Energies: A Viable Approach Beyond Nobleâ€Metal Catalysts?. ChemElectroChem, 2021, 8, 46-48.	1.7	19
12	Method to Construct Volcano Relations by Multiscale Modeling: Building Bridges between the Catalysis and Biosimulation Communities. Journal of Physical Chemistry B, 2021, 125, 2098-2104.	1.2	1
13	Why approximating electrocatalytic activity by a single freeâ€energy change is insufficient. Electrochimica Acta, 2021, 375, 137975.	2.6	42
14	A Universal Approach to Quantify Overpotential-Dependent Selectivity Trends for the Competing Oxygen Evolution and Peroxide Formation Reactions: A Case Study on Graphene Model Electrodes. Journal of Physical Chemistry C, 2021, 125, 10413-10421.	1.5	9
15	The Sabatier Principle in Electrocatalysis: Basics, Limitations, and Extensions. Frontiers in Energy Research, 2021, 9, .	1.2	175
16	Why the breaking of the OOH versus OH scaling relation might cause decreased electrocatalytic activity. Chem Catalysis, 2021, 1, 258-271.	2.9	30
17	On the Lattice Oxygen Evolution Mechanism: Avoiding Pitfalls. ChemCatChem, 2021, 13, 4066-4074.	1.8	22
18	Why the optimum thermodynamic free-energy landscape of the oxygen evolution reaction reveals an asymmetric shape. Materials Today Energy, 2021, 21, 100831.	2.5	12

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19	General Efficacy of Atomically Dispersed Pt Catalysts for the Chlorine Evolution Reaction: Potential-Dependent Switching of the Kinetics and Mechanism. ACS Catalysis, 2021, 11, 12232-12246.	5.5	40
20	The electrochemical-step asymmetry index. MethodsX, 2021, 8, 101590.	0.7	4
21	Beyond thermodynamic-based material-screening concepts: Kinetic scaling relations exemplified by the chlorine evolution reaction over transition-metal oxides. Electrochimica Acta, 2020, 334, 135555.	2.6	15
22	Electrolyte Engineering as a Key Strategy Towards a Sustainable Energy Scenario?. ChemElectroChem, 2020, 7, 594-595.	1.7	5
23	Comparison of the Conventional Volcano Analysis with a Unifying Approach: Material Screening Based on a Combination of Experiment and Theory. Journal of Physical Chemistry C, 2020, 124, 822-828.	1.5	22
24	A Universal Descriptor for the Screening of Electrode Materials for Multiple-Electron Processes: Beyond the Thermodynamic Overpotential. ACS Catalysis, 2020, 10, 12607-12617.	5.5	91
25	Recent Progress in the Development of Screening Methods to Identify Electrode Materials for the Oxygen Evolution Reaction. Advanced Functional Materials, 2020, 30, 2005060.	7.8	49
26	Paradigm change in hydrogen electrocatalysis: The volcano's apex is located at weak bonding of the reaction intermediate. International Journal of Hydrogen Energy, 2020, 45, 27221-27229.	3.8	46
27	Design criteria for the competing chlorine and oxygen evolution reactions: avoid the OCl adsorbate to enhance chlorine selectivity. Physical Chemistry Chemical Physics, 2020, 22, 22451-22458.	1.3	41
28	Identifying a gold nanoparticle as a proactive carrier for transport of a doxorubicin-peptide complex. Colloids and Surfaces B: Biointerfaces, 2020, 194, 111155.	2.5	5
29	Does a Thermoneutral Electrocatalyst Correspond to the Apex of a Volcano Plot for a Simple Twoâ€Electron Process?. Angewandte Chemie - International Edition, 2020, 59, 10236-10240.	7.2	85
30	Does a Thermoneutral Electrocatalyst Correspond to the Apex of a Volcano Plot for a Simple Twoâ€Electron Process?. Angewandte Chemie, 2020, 132, 10320-10324.	1.6	14
31	Overpotentialâ€Dependent Volcano Plots to Assess Activity Trends in the Competing Chlorine and Oxygen Evolution Reactions. ChemElectroChem, 2020, 7, 1448-1455.	1.7	25
32	Beyond Dimensionally Stable Anodes: Singleâ€Atom Catalysts with Superior Chlorine Selectivity. ChemElectroChem, 2020, 7, 1528-1530.	1.7	12
33	Universality in Oxygen Evolution Electrocatalysis: Highâ€Throughput Screening and a Priori Determination of the Rateâ€Determining Reaction Step. ChemCatChem, 2020, 12, 2000-2003.	1.8	20
34	Design Criteria for Oxygen Evolution Electrocatalysts from First Principles: Introduction of a Unifying Material-Screening Approach. ACS Applied Energy Materials, 2019, 2, 7991-8001.	2.5	59
35	Beyond the Rate-Determining Step in the Oxygen Evolution Reaction over a Single-Crystalline IrO₂(110) Model Electrode: Kinetic Scaling Relations. ACS Catalysis, 2019, 9, 6755-6765.	5.5	117
36	Controlling Stability and Selectivity in the Competing Chlorine and Oxygen Evolution Reaction over Transition Metal Oxide Electrodes. ChemElectroChem, 2019, 6, 3401-3409.	1.7	57

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37	Beyond the Traditional Volcano Concept: Overpotential-Dependent Volcano Plots Exemplified by the Chlorine Evolution Reaction over Transition-Metal Oxides. Journal of Physical Chemistry C, 2019, 123, 16921-16928.	1.5	50
38	Activityâ€Stability Volcano Plots for Material Optimization in Electrocatalysis. ChemCatChem, 2019, 11, 3234-3241.	1.8	15
39	Is Thermodynamics a Good Descriptor for the Activity? Re-Investigation of Sabatierâ€™s Principle by the Free Energy Diagram in Electrocatalysis. ACS Catalysis, 2019, 9, 5320-5329.	5.5	94
40	Recent Advancements Towards Closing the Gap between Electrocatalysis and Battery Science Communities: The Computational Lithium Electrode and Activityâ€“Stability Volcano Plots. ChemSusChem, 2019, 12, 2330-2344.	3.6	33
41	Kinetic study of gold nanoparticles synthesized in the presence of chitosan and citric acid. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2018, 557, 106-115.	2.3	24
42	A Universal Approach To Determine the Free Energy Diagram of an Electrocatalytic Reaction. ACS Catalysis, 2018, 8, 1864-1879.	5.5	128
43	Activity â€“ Stability Volcano Plots for the Investigation of Nanoâ€Sized Electrode Materials in Lithiumâ€Ion Batteries. ChemElectroChem, 2018, 5, 3243-3248.	1.7	16
44	A short perspective of modeling electrode materials in lithium-ion batteries by the ab initio atomistic thermodynamics approach. Journal of Solid State Electrochemistry, 2018, 22, 3111-3117.	1.2	14
45	Temperature-Dependent Kinetic Studies of the Chlorine Evolution Reaction over RuO₂(110) Model Electrodes. ACS Catalysis, 2017, 7, 2403-2411.	5.5	111
46	Kinetics of Electrocatalytic Reactions from First-Principles: A Critical Comparison with the Ab Initio Thermodynamics Approach. Accounts of Chemical Research, 2017, 50, 1240-1247.	7.6	133
47	Constrained Ab Initio Thermodynamics: Transferring the Concept of Surface Pourbaix Diagrams in Electrocatalysis to Electrode Materials in Lithiumâ€Ion Batteries. ChemElectroChem, 2017, 4, 3231-3237.	1.7	27
48	Full Free Energy Diagram of an Electrocatalytic Reaction over a Singleâ€Crystalline Model Electrode. ChemElectroChem, 2017, 4, 2902-2908.	1.7	27
49	Full Kinetics from First Principles of the Chlorine Evolution Reaction over a RuO₂(110) Model Electrode. Angewandte Chemie - International Edition, 2016, 55, 7501-7504.	7.2	120
50	Full Kinetics from First Principles of the Chlorine Evolution Reaction over a RuO₂(110) Model Electrode. Angewandte Chemie, 2016, 128, 7627-7630.	1.6	15
51	Combined experiment and theory approach in surface chemistry: Stairway to heaven?. Surface Science, 2015, 640, 165-180.	0.8	22
52	Ligand Effects and Their Impact on Electrocatalytic Processes Exemplified with the Oxygen Evolution Reaction (OER) on RuO₂(110). ChemElectroChem, 2015, 2, 707-713.	1.7	64
53	Microscopic Insights into the Chlorine Evolution Reaction on RuO2(110): a Mechanistic Ab Initio Atomistic Thermodynamics Study. Electrocatalysis, 2015, 6, 163-172.	1.5	27
54	Chlorine Evolution Reaction on RuO2(110): Ab initio Atomistic Thermodynamics Study - Pourbaix Diagrams. Electrochimica Acta, 2014, 120, 460-466.	2.6	95

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55	Controlling Selectivity in the Chlorine Evolution Reaction over RuO₂â€Based Catalysts. Angewandte Chemie - International Edition, 2014, 53, 11032-11035.	7.2	182
56	On the optimum binding energy for the hydrogen evolution reaction: How do experiments contribute?. Electrochemical Science Advances, 0, , e2100101.	1.2	1