Vitaly Alexandrov

List of Publications by Year in descending order

43 papers	1,701 citations	257450 24 h-index	276875 41 g-index
43 all docs	43 docs citations	43 times ranked	2201 citing authors

#	Article	IF	Citations
1	Role of Defects in the Interplay between Adsorbate Evolving and Lattice Oxygen Mechanisms of the Oxygen Evolution Reaction in RuO₂ and IrO₂. ACS Catalysis, 2020, 10, 3650-3657.	11.2	339
2	Poly-Amide Modified Copper Foam Electrodes for Enhanced Electrochemical Reduction of Carbon Dioxide. ACS Catalysis, 2018, 8, 4132-4142.	11.2	165
3	Role of Dissolution Intermediates in Promoting Oxygen Evolution Reaction at RuO₂(110) Surface. Journal of Physical Chemistry C, 2019, 123, 22151-22157.	3.1	86
4	Increased Irâ€“Ir Interaction in Iridium Oxide during the Oxygen Evolution Reaction at High Potentials Probed by Operando Spectroscopy. ACS Catalysis, 2021, 11, 10043-10057.	11.2	75
5	Mechanistic Study of IrO₂ Dissolution during the Electrocatalytic Oxygen Evolution Reaction. Journal of Physical Chemistry Letters, 2020, 11, 2695-2700.	4.6	70
6	Ab initio modeling of Fe(<scp>ii</scp>) adsorption and interfacial electron transfer at goethite (Î±-FeOOH) surfaces. Physical Chemistry Chemical Physics, 2015, 17, 14518-14531.	2.8	60
7	Effect of intrinsic point defects on ferroelectric polarization behavior of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m Physical Review B, 2017, 95, .	3.2	57
8	Ab Initio Thermodynamics and Kinetics of the Lattice Oxygen Evolution Reaction in Iridium Oxides. ACS Energy Letters, 2021, 6, 1124-1133.	17.4	56
9	Insights into the Mechanism of Fe(II) Adsorption and Oxidation at Feâ€“Clay Mineral Surfaces from First-Principles Calculations. Journal of Physical Chemistry C, 2013, 117, 22880-22886.	3.1	53
10	Electron Exchange and Conduction in Nontronite from First-Principles. Journal of Physical Chemistry C, 2013, 117, 2032-2040.	3.1	43
11	Electron transport in pure and substituted iron oxyhydroxides by small-polaron migration. Journal of Chemical Physics, 2014, 140, 234701.	3.0	43
12	Effects of Strain and Film Thickness on the Stability of the Rhombohedral Phase of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Hf</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Applied, 2020, 14, .	3.8	43
13	Periodicity in the Electrochemical Dissolution of Transition Metals. Angewandte Chemie - International Edition, 2021, 60, 13343-13349.	13.8	40
14	Defect-Assisted Tunneling Electroresistance in Ferroelectric Tunnel Junctions. Physical Review Letters, 2018, 121, 056601.	7.8	39
15	Actinide Dioxides in Water: Interactions at the Interface. Journal of Physical Chemistry Letters, 2011, 2, 3130-3134.	4.6	38
16	First-principles study of adsorptionâ€“desorption kinetics of aqueous V²⁺/V³⁺ redox species on graphite in a vanadium redox flow battery. Physical Chemistry Chemical Physics, 2017, 19, 14897-14901.	2.8	38
17	Iron Dissolution from Goethite (Î±-FeOOH) Surfaces in Water by Ab Initio Enhanced Free-Energy Simulations. Journal of Physical Chemistry C, 2018, 122, 16086-16091.	3.1	33
18	A combined theoretical-experimental study of interactions between vanadium ions and Nafion membrane in all-vanadium redox flow batteries. Journal of Power Sources, 2018, 373, 150-160.	7.8	32

#	ARTICLE	IF	CITATIONS
19	Tunneling Hot Spots in Ferroelectric SrTiO₃. Nano Letters, 2018, 18, 491-497.	9.1	30
20	Ab Initio Modeling of Transition Metal Dissolution from the LiNi_{0.5}Mn_{1.5}O₄ Cathode. ACS Applied Materials & Interfaces, 2019, 11, 20110-20116.	8.0	30
21	Ab Initio Thermodynamics of Iridium Surface Oxidation and Oxygen Evolution Reaction. Journal of Physical Chemistry C, 2018, 122, 29350-29358.	3.1	28
22	Ab Initio Metadynamics Study of the VO₂⁺/VO²⁺ Redox Reaction Mechanism at the Graphite Edge/Water Interface. ACS Applied Materials & Interfaces, 2018, 10, 20621-20626.	8.0	27
23	Ab Initio Modeling of Bulk and Intragranular Diffusion in Ni Alloys. Journal of Physical Chemistry Letters, 2015, 6, 1618-1623.	4.6	26
24	Structure, hydrolysis, and diffusion of aqueous vanadium ions from Car-Parrinello molecular dynamics. Journal of Chemical Physics, 2016, 145, 114303.	3.0	26
25	CO₂ Adsorption and Reactivity on Rutile TiO₂(110) in Water: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 10476-10483.	3.1	23
26	Ferroelectric Tunnel Junctions Enhanced by a Polar Oxide Barrier Layer. Nano Letters, 2019, 19, 7385-7393.	9.1	23
27	Mechanistic Theoretical Investigation of Self-Discharge Reactions in a Vanadium Redox Flow Battery. Journal of Physical Chemistry B, 2019, 123, 3976-3983.	2.6	23
28	First-principles computational study of defect clustering in solid solutions of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ThO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms trivalent oxides. Physical Review B, 2010, 82, .	3.2	20
29	Energetics of mixing in ThO2â€“CeO2 fluorite solid solutions. Journal of Nuclear Materials, 2011, 419, 72-75.	2.7	16
30	Electrocatalytic Activity of Oxygen-Functionalized Carbon Electrodes for Vanadium Redox Flow Batteries from Free-Energy Calculations. ACS Applied Energy Materials, 2020, 3, 7543-7549.	5.1	16
31	Magnetoelectric Effect at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Ni</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mi>Hf</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> Interface Induced by Ferroelectric Polarization. Physical Review Applied, 2019, 12, .	3.8	15
32	Adsorption and diffusion of atomic oxygen and sulfur at pristine and doped Ni surfaces with implications for stress corrosion cracking. Corrosion Science, 2016, 113, 26-30.	6.6	14
33	Theoretical Insights into Oxidation States of Transition Metals at (001) and (111) LiNi0.5Mn1.5O4Spinel Surfaces. Journal of the Electrochemical Society, 2018, 165, A1099-A1103.	2.9	14
34	First-Principles Modeling of Oxygen Interaction with SrTiO₃(001) Surface: Comparative Density-Functional LCAO and Plane-Wave Study. Integrated Ferroelectrics, 2011, 123, 10-17.	0.7	11
35	Multiscale model of metal alloy oxidation at grain boundaries. Journal of Chemical Physics, 2015, 142, 214114.	3.0	10
36	Theoretical study of mixing energetics in homovalent fluorite-structured oxide solid solutions. Journal of Nuclear Materials, 2014, 444, 292-297.	2.7	8

#	Article	IF	Citations
37	Revealing Elusive Intermediates of Platinum Cathodic Corrosion through DFT Simulations. Journal of Physical Chemistry Letters, 2022, 13, 3047-3052.	4.6	8
38	Enhancing Oxygen Electroreduction Activity of Single-Site Feâ€“Nâ€“C Catalysts by a Metal Support. Journal of Physical Chemistry C, 2019, 123, 30335-30340.	3.1	6
39	Structure-Dependent Electrical Double-Layer Capacitances of the Basal Plane Pd(hkl) Electrodes in HClO₄. Journal of Physical Chemistry C, 2022, 126, 11414-11420.	3.1	5
40	Kinetics of pHâ€dependent interactions between PDâ€1 and PDâ€L1 immune checkpoint proteins from molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1162-1168.	2.6	4
41	Molecular-Level Control over Ionic Conduction and Ionic Current Direction by Designing Macrocycle-Based Ionomers. Jacs Au, 2022, 2, 1144-1159.	7.9	4
42	Periodicity in the Electrochemical Dissolution of Transition Metals. Angewandte Chemie, 2021, 133, 13455-13461.	2.0	3
43	Layer-By-Layer Polyelectrolyte Assembly for the Protection of GaP Surfaces from Photocorrosion. ACS Applied Nano Materials, 2021, 4, 425-431.	5.0	1