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	Revealing Elusive Intermediates of Platinum Cathodic Corrosion through DFT Simulations. Journal of Physical Chemistry Letters, 2022, 13, 3047-3052.	4.6	8
2	Molecular-Level Control over Ionic Conduction and Ionic Current Direction by Designing Macrocycle-Based Ionomers. Jacs Au, 2022, 2, 1144-1159.	7.9	4
3	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
4	Ab Initio Thermodynamics and Kinetics of the Lattice Oxygen Evolution Reaction in Iridium Oxides. ACS Energy Letters, 2021, 6, 1124-1133.	17.4	56
5	Periodicity in the Electrochemical Dissolution of Transition Metals. Angewandte Chemie - International Edition, 2021, 60, 13343-13349.	13.8	40
6	Periodicity in the Electrochemical Dissolution of Transition Metals. Angewandte Chemie, 2021, 133, 13455-13461.	2.0	3
7	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
8	Layer-By-Layer Polyelectrolyte Assembly for the Protection of GaP Surfaces from Photocorrosion. ACS Applied Nano Materials, 2021, 4, 425-431.	5.0	1
9	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
10	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
11	Mechanistic Study of IrO₂ Dissolution during the Electrocatalytic Oxygen Evolution Reaction. Journal of Physical Chemistry Letters, 2020, 11, 2695-2700.	4.6	70
12	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
13	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
14	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
15	Ferroelectric Tunnel Junctions Enhanced by a Polar Oxide Barrier Layer. Nano Letters, 2019, 19, 7385-7393.	9.1	23
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	Poly-Amide Modified Copper Foam Electrodes for Enhanced Electrochemical Reduction of Carbon Dioxide. ACS Catalysis, 2018, 8, 4132-4142.	11.2	165
21	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
22	Tunneling Hot Spots in Ferroelectric SrTiO₃. Nano Letters, 2018, 18, 491-497.	9.1	30
23	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
24	Ab Initio Thermodynamics of Iridium Surface Oxidation and Oxygen Evolution Reaction. Journal of Physical Chemistry C, 2018, 122, 29350-29358.	3.1	28
25	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
26	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
27	Defect-Assisted Tunneling Electroresistance in Ferroelectric Tunnel Junctions. Physical Review Letters, 2018, 121, 056601.	7.8	39
28	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	37
29	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
30	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
31	Structure, hydrolysis, and diffusion of aqueous vanadium ions from Car-Parrinello molecular dynamics. Journal of Chemical Physics, 2016, 145, 114303.	3.0	26
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	Multiscale model of metal alloy oxidation at grain boundaries. Journal of Chemical Physics, 2015, 142, 214114.	3.0	10
34	Ab Initio Modeling of Bulk and Intragranular Diffusion in Ni Alloys. Journal of Physical Chemistry Letters, 2015, 6, 1618-1623.	4.6	26
35	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
36	Electron transport in pure and substituted iron oxyhydroxides by small-polaron migration. Journal of Chemical Physics, 2014, 140, 234701.	3.0	43

#	Article	IF	Citations
37	Theoretical study of mixing energetics in homovalent fluorite-structured oxide solid solutions. Journal of Nuclear Materials, 2014, 444, 292-297.	2.7	8
38	Electron Exchange and Conduction in Nontronite from First-Principles. Journal of Physical Chemistry C, 2013, 117, 2032-2040.	3.1	43
39	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
40	Actinide Dioxides in Water: Interactions at the Interface. Journal of Physical Chemistry Letters, 2011, 2, 3130-3134.	4.6	38
41	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
42	Energetics of mixing in ThO2â€“CeO2 fluorite solid solutions. Journal of Nuclear Materials, 2011, 419, 72-75.	2.7	16
43	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