Wissam A Saidi

List of Publications by Year
in descending order

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126 papers	4,327 citations	101384 36 h-index	133063 59 g-index
129 all docs	129 docs citations	129 times ranked	5773 citing authors

#	Article	IF	Citations
1	Dimensional Control over Metal Halide Perovskite Crystallization Guided by Active Learning. Chemistry of Materials, 2022, 34, 756-767.	3.2	13
2	Uneven Oxidation and Surface Reconstructions on Stepped Cu(100) and Cu(110). Nano Letters, 2022, 22, 1075-1082.	4.5	9
3	Convergence acceleration in machine learning potentials for atomistic simulations. , 2022, 1, 61-69.		18
4	Controlling the nucleation and growth of ultrasmall metal nanoclusters with MoS₂ grain boundaries. Nanoscale, 2022, 14, 617-625.	2.8	7
5	Optimizing the Catalytic Activity of Pd-Based Multinary Alloys toward Oxygen Reduction Reaction. Journal of Physical Chemistry Letters, 2022, 13, 1042-1048.	2.1	17
6	Universally characterizing atomistic strain via simulation, statistics, and machine learning: Low-angle grain boundaries. Acta Materialia, 2022, 226, 117635.	3.8	5
7	â€œSelf-trappingâ€•in solar cell hybrid inorganic-organic perovskite absorbers. Applied Materials Today, 2022, 26, 101380.	2.3	6
8	Hydrogen localization and cluster formation in Î±-Zr from first-principles investigations. Computational Materials Science, 2022, 209, 111384.	1.4	3
9	Emergence of local scaling relations in adsorption energies on high-entropy alloys. Npj Computational Materials, 2022, 8, .	3.5	18
10	Electron-Volt Fluctuation of Defect Levels in Metal Halide Perovskites on a 100 ps Time Scale. Journal of Physical Chemistry Letters, 2022, 13, 5946-5952.	2.1	18
11	Reconciling the Volcano Trend with the Butlerâ€“Volmer Model for the Hydrogen Evolution Reaction. Journal of Physical Chemistry Letters, 2022, 13, 5310-5315.	2.1	10
12	Atomistic Mechanisms of Binary Alloy Surface Segregation from Nanoseconds to Seconds Using Accelerated Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 4447-4455.	2.3	3
13	Applicability of Allenâ€“Heineâ€“Cardona Theory on MO_x Metal Oxides and ABO₃ Perovskites: Toward High-Temperature Optoelectronic Applications. Chemistry of Materials, 2022, 34, 6108-6115.	3.2	7
14	Revisiting trends in the exchange current for hydrogen evolution. Catalysis Science and Technology, 2021, 11, 6832-6838.	2.1	21
15	Size-dependent polarizabilities and van der Waals dispersion coefficients of fullerenes from large-scale complex polarization propagator calculations. Journal of Chemical Physics, 2021, 154, 074304.	1.2	5
16	Revealing High-Temperature Reduction Dynamics of High-Entropy Alloy Nanoparticles via In Situ Transmission Electron Microscopy. Nano Letters, 2021, 21, 1742-1748.	4.5	26
17	Real-time GW -BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide. Science Advances, 2021, 7, .	4.7	70
18	Tuning electrical and interfacial thermal properties of bilayer MoS₂ via electrochemical intercalation. Nanotechnology, 2021, 32, 265202.	1.3	3

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19	Assessing the Effects of Temperature and Oxygen Vacancy on Band Gap Renormalization in LaCrO_{3â^Î´}: First-Principles and Experimental Corroboration. ACS Applied Materials & Interfaces, 2021, 13, 17717-17725.	4.0	18
20	Optimization of High-Entropy Alloy Catalyst for Ammonia Decomposition and Ammonia Synthesis. Journal of Physical Chemistry Letters, 2021, 12, 5185-5192.	2.1	46
21	Unusual layer-by-layer growth of epitaxial oxide islands during Cu oxidation. Nature Communications, 2021, 12, 2781.	5.8	27
22	Universal prediction of strain footprints via simulation, statistics, and machine learning: low-Î£ grain boundaries. Acta Materialia, 2021, 211, 116850.	3.8	5
23	Robust, Multi-Length-Scale, Machine Learning Potential for Agâ€“Au Bimetallic Alloys from Clusters to Bulk Materials. Journal of Physical Chemistry C, 2021, 125, 17438-17447.	1.5	31
24	Improved Al-Mg alloy surface segregation predictions with a machine learning atomistic potential. Physical Review Materials, 2021, 5, .	0.9	18
25	Thermal fluctuations and carrier localization induced by dynamic disorder in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>MAPbI</mml:mi></mml:mrow><mml:mn>3</ described by first-principles based tight-binding model. Physical Review Materials, 2021, 5, .	3.1	2
26	Grain Boundaries in Methylammonium Lead Halide Perovskites Facilitate Water Diffusion. Advanced Energy and Sustainability Research, 2021, 2, 2100087.	2.8	9
27	Quantifying Temperature Dependence of Electronic Band Gaps and Optical Properties in SnO₂ and SnO via First-Principles Simulations. Journal of Physical Chemistry C, 2021, 125, 22231-22238.	1.5	9
28	Stability and electronic properties of two-dimensional metalâ€“organic perovskites in Janus phase. APL Materials, 2021, 9, 111105.	2.2	2
29	Identifying high-performance and durable methylammonium-free lead halide perovskites via high-throughput synthesis and characterization. Energy and Environmental Science, 2021, 14, 6638-6654.	15.6	20
30	Weak Anharmonicity Rationalizes the Temperature-Driven Acceleration of Nonradiative Dynamics in Cu₂ZnSnS₄Photoabsorbers. ACS Applied Materials & Interfaces, 2021, 13, 61365-61373.	4.0	11
31	Evaluating the accuracy of common Î³-Al2O3 structure models by selected area electron diffraction from high-quality crystalline Î³-Al2O3. Acta Materialia, 2020, 182, 257-266.	3.8	48
32	High Activity toward the Hydrogen Evolution Reaction on the Edges of MoS₂-Supported Platinum Nanoclusters Using Cluster Expansion and Electrochemical Modeling. Chemistry of Materials, 2020, 32, 1315-1321.	3.2	35
33	Diverse electronic properties of 2D layered Se-containing materials composed of quasi-1D atomic chains. Physical Chemistry Chemical Physics, 2020, 22, 2122-2129.	1.3	10
34	Origin and Suppression of Beam Damage-Induced Oxygen-K Edge Artifact from Î³-Al2O3 using Cryo-EELS. Ultramicroscopy, 2020, 219, 113127.	0.8	10
35	In Situ Oxidation Studies of High-Entropy Alloy Nanoparticles. ACS Nano, 2020, 14, 15131-15143.	7.3	71
36	First-principles exploration of oxygen vacancy impact on electronic and optical properties of ABO_{3â^Î´} (A = La, Sr; B = Cr, Mn) perovskites. Physical Chemistry Chemical Physics, 2020, 22, 27163-27172.	1.3	28

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37	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2020, 11, 10073-10080.	2.1	65
38	Long-Lived Hot Electron in a Metallic Particle for Plasmonics and Catalysis: Ab Initio Nonadiabatic Molecular Dynamics with Machine Learning. ACS Nano, 2020, 14, 10608-10615.	7.3	46
39	First-principles study of Pd-alloyed Cu(111) surface in hydrogen atmosphere at realistic temperatures. Journal of Applied Physics, 2020, 128, 145302.	1.1	2
40	Probing the Local Bonding at the Pt/Î³-Al₂O₃ Interface. Journal of Physical Chemistry C, 2020, 124, 9876-9885.	1.5	10
41	Theoretical and experimental study of temperature effect on electronic and optical properties of TiO₂: Comparing rutile and anatase. Journal of Physics Condensed Matter, 2020, 32, 405705.	0.7	5
42	Graphene Activation Explains the Enhanced Hydrogen Evolution on Graphene-Coated Molybdenum Carbide Electrocatalysts. Journal of Physical Chemistry Letters, 2020, 11, 2759-2764.	2.1	31
43	Iodine and Sulfur Vacancy Cooperation Promotes Ultrafast Charge Extraction at MAPbI₃/MoS₂ Interface. ACS Energy Letters, 2020, 5, 1346-1354.	8.8	53
44	Anharmonicity Explains Temperature Renormalization Effects of the Band Gap in SrTiO₃. Journal of Physical Chemistry Letters, 2020, 11, 2518-2523.	2.1	30
45	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. Science Advances, 2020, 6, eaaw7453.	4.7	182
46	In situ environmental TEM observation of two-stage shrinking of Cu₂O islands on Cu(100) during methanol reduction. Physical Chemistry Chemical Physics, 2020, 22, 2738-2742.	1.3	14
47	Soft Lattice and Defect Covalency Rationalize Tolerance of Î²â€CsPbI₃ Perovskite Solar Cells to Native Defects. Angewandte Chemie - International Edition, 2020, 59, 6435-6441.	7.2	147
48	Soft Lattice and Defect Covalency Rationalize Tolerance of Î²â€CsPbI₃ Perovskite Solar Cells to Native Defects. Angewandte Chemie, 2020, 132, 6497-6503.	1.6	8
49	Optimization and validation of a deep learning CuZr atomistic potential: Robust applications for crystalline and amorphous phases with near-DFT accuracy. Journal of Chemical Physics, 2020, 152, 154701.	1.2	35
50	Revealing Sintering Kinetics of MoS₂-Supported Metal Nanocatalysts in Atmospheric Gas Environments via Operando Transmission Electron Microscopy. ACS Nano, 2020, 14, 4074-4086.	7.3	15
51	Machine-learning structural and electronic properties of metal halide perovskites using a hierarchical convolutional neural network. Npj Computational Materials, 2020, 6, .	3.5	93
52	Atomic Scale Dynamic Process of Cu Oxidation Revealed By Correlated in situ Environmental TEM and DFT Simulations. Microscopy and Microanalysis, 2019, 25, 1494-1495.	0.2	1
53	In situ Atomic Scale Observation of Cu2O Reduction Under Methanol. Microscopy and Microanalysis, 2019, 25, 1866-1867.	0.2	2
54	Determination of the Crystal Structure of Gamma-Alumina by Electron Diffraction and Electron Energy-Loss Spectroscopy. Microscopy and Microanalysis, 2019, 25, 2036-2037.	0.2	1

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55	Connecting Oxide Nucleation and Growth to Oxygen Diffusion Energetics on Stepped Cu(011) Surfaces: An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 452-463.	1.5	19
56	Mechanism behind the Inhibiting Effect of CO₂ on the Oxidation of Alâ€“Mg Alloys. Industrial & Engineering Chemistry Research, 2019, 58, 1434-1442.	1.8	9
57	Room-temperature epitaxy of metal thin films on tungsten diselenide. Journal of Crystal Growth, 2019, 505, 44-51.	0.7	12
58	Delocalized Impurity Phonon Induced Electronâ€“Hole Recombination in Doped Semiconductors. Nano Letters, 2018, 18, 1592-1599.	4.5	86
59	Dependence of H2 and CO2 selectivity on Cu oxidation state during partial oxidation of methanol on Cu/ZnO. Applied Catalysis A: General, 2018, 556, 64-72.	2.2	34
60	Probing Dynamic Processes of the Initial Stages of Cu(100) Surface Oxidation by in situ Environmental TEM and Multiscale Simulations. Microscopy and Microanalysis, 2018, 24, 262-263.	0.2	4
61	Correlative Structure-Bonding and Stability Studies of Pt/Î³-Al2O3 Catalysts. Microscopy and Microanalysis, 2018, 24, 1644-1645.	0.2	1
62	Effects of Electronâ€“Phonon Coupling on Electronic Properties of Methylammonium Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 7090-7097.	2.1	44
63	Proton Migration in Hybrid Lead Iodide Perovskites: From Classical Hopping to Deep Quantum Tunneling. Journal of Physical Chemistry Letters, 2018, 9, 6536-6543.	2.1	15
64	First-Principles Investigations of the Temperature Dependence of Electronic Structure and Optical Properties of Rutile TiO₂. Journal of Physical Chemistry C, 2018, 122, 22642-22649.	1.5	18
65	Segregation induced order-disorder transition in Cu(Au) surface alloys. Acta Materialia, 2018, 154, 220-227.	3.8	11
66	Phonon-coupled ultrafast interlayer charge oscillation at van der Waals heterostructure interfaces. Physical Review B, 2018, 97, .	1.1	81
67	Tuning Solvated Electrons by Polarâ€“Nonpolar Oxide Heterostructure. Journal of Physical Chemistry Letters, 2018, 9, 3049-3056.	2.1	13
68	Experimentally Validated Structures of Supported Metal Nanoclusters on MoS₂. Journal of Physical Chemistry Letters, 2018, 9, 2972-2978.	2.1	23
69	In situstudy of nucleation and growth dynamics of Au nanoparticles on MoS₂nanoflakes. Nanoscale, 2018, 10, 15809-15818.	2.8	38
70	Superatom Molecular Orbital as an Interfacial Charge Separation State. Journal of Physical Chemistry Letters, 2018, 9, 3485-3490.	2.1	29
71	Tuning the hydrogen evolution activity of Î²-Mo₂C nanoparticles via control of their growth conditions. Nanoscale, 2017, 9, 3252-3260.	2.8	38
72	Effects of Cr-doping on the adsorption and dissociation of S, SO, and SO2 on Ni(111) surfaces. Journal of Chemical Physics, 2017, 146, 154701.	1.2	5

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73	Enhanced Mass Transfer in the Step Edge Induced Oxidation on Cu(100) Surface. Journal of Physical Chemistry C, 2017, 121, 11251-11260.	1.5	19
74	Role of Surface Stress on the Reactivity of Anatase TiO₂(001). Journal of Physical Chemistry Letters, 2017, 8, 1764-1771.	2.1	39
75	Defect-Induced Near-Infrared Photoluminescence of Single-Walled Carbon Nanotubes Treated with Polyunsaturated Fatty Acids. Journal of the American Chemical Society, 2017, 139, 4859-4865.	6.6	44
76	Structural Stabilities and Electronic Properties of High-Angle Grain Boundaries in Perovskite Cesium Lead Halides. Journal of Physical Chemistry C, 2017, 121, 1715-1722.	1.5	99
77	Comparison of Spinel and Monoclinic Crystal Structures of Î³-Al2O3 for Simulation of Electron Energy Loss Spectra. Microscopy and Microanalysis, 2017, 23, 2020-2021.	0.2	0
78	Constructing a Predictive Model of Copper Oxidation from Experiment and Theory. Microscopy and Microanalysis, 2017, 23, 920-921.	0.2	3
79	Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface. Nano Letters, 2017, 17, 6435-6442.	4.5	204
80	Structures of defects on anatase TiO₂(001) surfaces. Nanoscale, 2017, 9, 11553-11565.	2.8	28
81	Atomically Visualizing Elemental Segregation-Induced Surface Alloying and Restructuring. Journal of Physical Chemistry Letters, 2017, 8, 6035-6040.	2.1	10
82	Segregation of Native Defects to the Grain Boundaries in Methylammonium Lead Iodide Perovskite. Journal of Physical Chemistry Letters, 2017, 8, 5935-5942.	2.1	56
83	Facile Anhydrous Proton Transport on Hydroxyl Functionalized Graphane. Physical Review Letters, 2017, 118, 186101.	2.9	21
84	2D halide perovskite-based van der Waals heterostructures: contact evaluation and performance modulation. 2D Materials, 2017, 4, 035009.	2.0	23
85	Controlling nucleation, growth, and orientation of metal halide perovskite thin films with rationally selected additives. Journal of Materials Chemistry A, 2017, 5, 113-123.	5.2	115
86	Temperature Dependence of the Energy Levels of Methylammonium Lead Iodide Perovskite from First-Principles. Journal of Physical Chemistry Letters, 2016, 7, 5247-5252.	2.1	100
87	Polarizabilities and van der WaalsC6coefficients of fullerenes from an atomistic electrodynamics model: Anomalous scaling with number of carbon atoms. Journal of Chemical Physics, 2016, 145, 024311.	1.2	4
88	Nature of the cubic to tetragonal phase transition in methylammonium lead iodide perovskite. Journal of Chemical Physics, 2016, 145, 144702.	1.2	53
89	Early and transient stages of Cu oxidation: Atomistic insights from theoretical simulations and in situ experiments. Surface Science, 2016, 652, 98-113.	0.8	37
90	Tunability of the two-dimensional electron gas at the LaAlO₃/SrTiO₃ interface by strain-induced ferroelectricity. Physical Chemistry Chemical Physics, 2016, 18, 28474-28484.	1.3	25

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91	Ultrafast Dynamics of Photongenerated Holes at a CH₃OH/TiO₂ Rutile Interface. Journal of the American Chemical Society, 2016, 138, 13740-13749.	6.6	126
92	Hydrogen-induced atomic structure evolution of the oxygen-chemisorbed Cu(110) surface. Journal of Chemical Physics, 2016, 145, 234704.	1.2	7
93	Surface-Enhanced Raman Scattering Due to Charge-Transfer Resonances: A Time-Dependent Density Functional Theory Study of Ag₁₃-4-Mercaptopyridine. Journal of Physical Chemistry C, 2016, 120, 20721-20735.	1.5	31
94	Step-Edge Directed Metal Oxidation. Journal of Physical Chemistry Letters, 2016, 7, 2530-2536.	2.1	29
95	Nano-scale polarâ€“nonpolar oxide heterostructures for photocatalysis. Nanoscale, 2016, 8, 6057-6063.	2.8	14
96	Modified Schottky emission to explain thickness dependence and slow depolarization in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2015, 91, .	1.1	3
97	Investigation of the Structural and Electronic Properties of Pt/Î³-Al2O3, a Model Catalyst System. Microscopy and Microanalysis, 2015, 21, 1655-1656.	0.2	0
98	Step-Induced Oxygen Upward Diffusion on Stepped Cu(100) Surface. Journal of Physical Chemistry C, 2015, 119, 251-261.	1.5	21
99	Density Functional Theory Study of Nucleation and Growth of Pt Nanoparticles on MoS₂(001) Surface. Crystal Growth and Design, 2015, 15, 642-652.	1.4	32
100	Temperature dependent energy levels of methylammonium lead iodide perovskite. Applied Physics Letters, 2015, 106, .	1.5	159
101	Trends in the Adsorption and Growth Morphology of Metals on the MoS₂(001) Surface. Crystal Growth and Design, 2015, 15, 3190-3200.	1.4	46
102	Synthesis of {111}-Faceted Au Nanocrystals Mediated by Polyvinylpyrrolidone: Insights from Density-Functional Theory and Molecular Dynamics. Journal of Physical Chemistry C, 2015, 119, 11982-11990.	1.5	32
103	Origins of thermal conductivity changes in strained crystals. Physical Review B, 2014, 90, .	1.1	84
104	Influence of strain and metal thickness on metal-MoS2 contacts. Journal of Chemical Physics, 2014, 141, 094707.	1.2	37
105	Spectroscopic signatures of topological and diatom-vacancy defects in single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2014, 16, 1479-1486.	1.3	13
106	Effects of Topological Defects and Diatom Vacancies on Characteristic Vibration Modes and Raman Intensities of Zigzag Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2014, 118, 7235-7241.	1.1	10
107	Strong Reciprocal Interaction between Polarization and Surface Stoichiometry in Oxide Ferroelectrics. Nano Letters, 2014, 14, 6711-6717.	4.5	37
108	Role of oxygen in Cu(1 1 0) surface restructuring in the vicinity of step edges. Chemical Physics Letters, 2014, 613, 64-69.	1.2	15

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109	Surface-Step-Induced Oscillatory Oxide Growth. Physical Review Letters, 2014, 113, 136104.	2.9	52
110	Kinetic Barriers of the Phase Transition in the Oxygen Chemisorbed Cu(110)-(2 Ã— 1)-O as a Function of Oxygen Coverage. Journal of Physical Chemistry C, 2014, 118, 20858-20866.	1.5	24
111	Van der Waals Epitaxial Growth of Transition Metal Dichalcogenides on Pristine and N-Doped Graphene. Crystal Growth and Design, 2014, 14, 4920-4928.	1.4	17
112	Probing single-walled carbon nanotube defect chemistry using resonance Raman spectroscopy. Carbon, 2014, 67, 17-26.	5.4	27
113	Insight into the Mechanism of Graphene Oxide Degradation via the Photo-Fenton Reaction. Journal of Physical Chemistry C, 2014, 118, 10519-10529.	1.5	101
114	Coexisting Surface Phases and Coherent One-Dimensional Interfaces on BaTiO₃(001). ACS Nano, 2014, 8, 4465-4473.	7.3	20
115	Oxygen chemisorption-induced surface phase transitions on Cu(110). Surface Science, 2014, 627, 75-84.	0.8	40
116	TFOx: A versatile kinetic Monte Carlo program for simulations of island growth in three dimensions. Computational Materials Science, 2014, 91, 292-302.	1.4	9
117	Understanding the Adsorption of CuPc and ZnPc on Noble Metal Surfaces by Combining Quantum-Mechanical Modelling and Photoelectron Spectroscopy. Molecules, 2014, 19, 2969-2992.	1.7	69
118	Oxygen Reduction Electrocatalysis Using N-Doped Graphene Quantum-Dots. Journal of Physical Chemistry Letters, 2013, 4, 4160-4165.	2.1	132
119	Binding of Polyvinylpyrrolidone to Ag Surfaces: Insight into a Structure-Directing Agent from Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry C, 2013, 117, 1163-1171.	1.5	93
120	Comparison of the Binding of Polyvinylpyrrolidone and Polyethylene Oxide to Ag Surfaces: Elements of a Successful Structure-Directing Agent. Journal of Physical Chemistry C, 2013, 117, 11444-11448.	1.5	35
121	In situ atomic-scale visualization of oxide islanding during oxidation of Cu surfaces. Chemical Communications, 2013, 49, 10862.	2.2	54
122	Understanding Structure and Bonding of Multilayered Metalâ€“Organic Nanostructures. Journal of Physical Chemistry C, 2013, 117, 3055-3061.	1.5	36
123	The Effect of Metal Catalyst on the Electrocatalytic Activity of Nitrogen-Doped Carbon Nanotubes. Journal of Physical Chemistry C, 2013, 117, 25213-25221.	1.5	36
124	Non-additivity of polarizabilities and van der Waals C6 coefficients of fullerenes. Journal of Chemical Physics, 2013, 138, 114107.	1.2	34
125	Atomic and Electronic Structure of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>(001)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo		