Wissam A Saidi

List of Publications by Year in Descending Order

117 papers	2,789 citations	29 h-index	47 g-index
129 ext. papers	3,490 ext. citations	6.3 avg, IF	6.02 L-index

#	Paper	IF	Citations
117	Dimensional Control over Metal Halide Perovskite Crystallization Guided by Active Learning. *Chemistry of Materials*, **2022**, 34, 756-767	9.6	3
116	Optimizing the Catalytic Activity of Pd-Based Multinary Alloys toward Oxygen Reduction Reaction.. *Journal of Physical Chemistry Letters*, **2022**, 1042-1048	6.4	3
115	Universally characterizing atomistic strain via simulation, statistics, and machine learning: Low-angle grain boundaries. *Acta Materialia*, **2022**, 226, 117635	8.4	0
114	Self-trapping in solar cell hybrid inorganic-organic perovskite absorbers. *Applied Materials Today*, **2022**, 26, 101380	6.6	0
113	Hydrogen localization and cluster formation in Zr from first-principles investigations. *Computational Materials Science*, **2022**, 209, 111384	3.2	0
112	Stability and electronic properties of two-dimensional metal-organic perovskites in Janus phase. *APL Materials*, **2021**, 9, 111105	5.7	1
111	Identifying high-performance and durable methylammonium-free lead halide perovskites via high-throughput synthesis and characterization. *Energy and Environmental Science*, **2021**, 14, 6638-6654	35.4	4
110	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	3.8	0
109	Real-time -BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide. *Science Advances*, **2021**, 7,	14.3	23
108	Assessing the Effects of Temperature and Oxygen Vacancy on Band Gap Renormalization in LaCrO: First-Principles and Experimental Corroboration. *ACS Applied Materials & Interfaces*, **2021**, 13, 17717-17725	9.5	7
107	Optimization of High-Entropy Alloy Catalyst for Ammonia Decomposition and Ammonia Synthesis. *Journal of Physical Chemistry Letters*, **2021**, 12, 5185-5192	6.4	8
106	Unusual layer-by-layer growth of epitaxial oxide islands during Cu oxidation. *Nature Communications*, **2021**, 12, 2781	17.4	7
105	Universal prediction of strain footprints via simulation, statistics, and machine learning: low-grain boundaries. *Acta Materialia*, **2021**, 211, 116850	8.4	3
104	Robust, Multi-Length-Scale, Machine Learning Potential for AgAu Bimetallic Alloys from Clusters to Bulk Materials. *Journal of Physical Chemistry C*, **2021**, 125, 17438-17447	3.8	9
103	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	3.9	1
102	Revealing High-Temperature Reduction Dynamics of High-Entropy Alloy Nanoparticles Transmission Electron Microscopy. *Nano Letters*, **2021**, 21, 1742-1748	11.5	8
101	Improved Al-Mg alloy surface segregation predictions with a machine learning atomistic potential. *Physical Review Materials*, **2021**, 5,	3.2	4

100	Weak Anharmonicity Rationalizes the Temperature-Driven Acceleration of Nonradiative Dynamics in CuZnSnS Photoabsorbers.. *ACS Applied Materials & Interfaces*, **2021**, 13, 61365-61373	9.5	3
99	First-principles study of Pd-alloyed Cu(111) surface in hydrogen atmosphere at realistic temperatures. *Journal of Applied Physics*, **2020**, 128, 145302	2.5	0
98	Probing the Local Bonding at the Pt/Al2O3 Interface. *Journal of Physical Chemistry C*, **2020**, 124, 9876-9885	3.7	3
97	Theoretical and experimental study of temperature effect on electronic and optical properties of TiO: comparing rutile and anatase. *Journal of Physics Condensed Matter*, **2020**, 32, 405705	1.8	2
96	Graphene Activation Explains the Enhanced Hydrogen Evolution on Graphene-Coated Molybdenum Carbide Electrocatalysts. *Journal of Physical Chemistry Letters*, **2020**, 11, 2759-2764	6.4	14
95	Iodine and Sulfur Vacancy Cooperation Promotes Ultrafast Charge Extraction at MAPbI3/MoS2 Interface. *ACS Energy Letters*, **2020**, 5, 1346-1354	20.1	29
94	Anharmonicity Explains Temperature Renormalization Effects of the Band Gap in SrTiO. *Journal of Physical Chemistry Letters*, **2020**, 11, 2518-2523	6.4	14
93	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. *Science Advances*, **2020**, 6, eaaw7453	14.3	99
92	In situ environmental TEM observation of two-stage shrinking of CuO islands on Cu(100) during methanol reduction. *Physical Chemistry Chemical Physics*, **2020**, 22, 2738-2742	3.6	4
91	Soft Lattice and Defect Covalency Rationalize Tolerance of CsPbI Perovskite Solar Cells to Native Defects. *Angewandte Chemie - International Edition*, **2020**, 59, 6435-6441	16.4	72
90	Soft Lattice and Defect Covalency Rationalize Tolerance of CsPbI3 Perovskite Solar Cells to Native Defects. *Angewandte Chemie*, **2020**, 132, 6497-6503	3.6	6
89	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, 154704	3.9	12
88	Revealing Sintering Kinetics of MoS-Supported Metal Nanocatalysts in Atmospheric Gas Environments Transmission Electron Microscopy. *ACS Nano*, **2020**, 14, 4074-4086	16.7	9
87	Evaluating the accuracy of common Al2O3 structure models by selected area electron diffraction from high-quality crystalline Al2O3. *Acta Materialia*, **2020**, 182, 257-266	8.4	19
86	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	9.6	14
85	Diverse electronic properties of 2D layered Se-containing materials composed of quasi-1D atomic chains. *Physical Chemistry Chemical Physics*, **2020**, 22, 2122-2129	3.6	4
84	Origin and Suppression of Beam Damage-Induced Oxygen-K Edge Artifact from AlO using Cryo-EELS. *Ultramicroscopy*, **2020**, 219, 113127	3.1	1
83	Oxidation Studies of High-Entropy Alloy Nanoparticles. *ACS Nano*, **2020**, 14, 15131-15143	16.7	22

82	First-principles exploration of oxygen vacancy impact on electronic and optical properties of ABO (A = La, Sr; B = Cr, Mn) perovskites. *Physical Chemistry Chemical Physics*, **2020**, 22, 27163-27172	3.6	10
81	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. *Journal of Physical Chemistry Letters*, **2020**, 11, 10073-10080	6.4	32
80	Long-Lived Hot Electron in a Metallic Particle for Plasmonics and Catalysis: Nonadiabatic Molecular Dynamics with Machine Learning. *ACS Nano*, **2020**, 14, 10608-10615	16.7	23
79	Machine-learning structural and electronic properties of metal halide perovskites using a hierarchical convolutional neural network. *Npj Computational Materials*, **2020**, 6,	10.9	39
78	Determination of the Crystal Structure of Gamma-Alumina by Electron Diffraction and Electron Energy-Loss Spectroscopy. *Microscopy and Microanalysis*, **2019**, 25, 2036-2037	0.5	1
77	Atomic Scale Dynamic Process of Cu Oxidation Revealed By Correlated in situ Environmental TEM and DFT Simulations. *Microscopy and Microanalysis*, **2019**, 25, 1494-1495	0.5	1
76	In situ Atomic Scale Observation of Cu2O Reduction Under Methanol. *Microscopy and Microanalysis*, **2019**, 25, 1866-1867	0.5	1
75	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	3.8	13
74	Mechanism behind the Inhibiting Effect of CO2 on the Oxidation of Al Mg Alloys. *Industrial & Engineering Chemistry Research*, **2019**, 58, 1434-1442	3.9	7
73	Room-temperature epitaxy of metal thin films on tungsten diselenide. *Journal of Crystal Growth*, **2019**, 505, 44-51	1.6	8
72	Delocalized Impurity Phonon Induced Electron-Hole Recombination in Doped Semiconductors. *Nano Letters*, **2018**, 18, 1592-1599	11.5	63
71	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	5.1	19
70	In situ study of nucleation and growth dynamics of Au nanoparticles on MoS nanoflakes. *Nanoscale*, **2018**, 10, 15809-15818	7.7	28
69	Superatom Molecular Orbital as an Interfacial Charge Separation State. *Journal of Physical Chemistry Letters*, **2018**, 9, 3485-3490	6.4	24
68	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	0.5	4
67	Correlative Structure-Bonding and Stability Studies of Pt/Al2O3 Catalysts. *Microscopy and Microanalysis*, **2018**, 24, 1644-1645	0.5	1
66	Effects of Electron-Phonon Coupling on Electronic Properties of Methylammonium Lead Iodide Perovskites. *Journal of Physical Chemistry Letters*, **2018**, 9, 7090-7097	6.4	27
65	Proton Migration in Hybrid Lead Iodide Perovskites: From Classical Hopping to Deep Quantum Tunneling. *Journal of Physical Chemistry Letters*, **2018**, 9, 6536-6543	6.4	10

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	3.8	6
63	Segregation induced order-disorder transition in Cu(Au) surface alloys. *Acta Materialia*, **2018**, 154, 220-227	7.4	7
62	Phonon-coupled ultrafast interlayer charge oscillation at van der Waals heterostructure interfaces. *Physical Review B*, **2018**, 97,	3.3	51
61	Tuning Solvated Electrons by Polar-Nonpolar Oxide Heterostructure. *Journal of Physical Chemistry Letters*, **2018**, 9, 3049-3056	6.4	11
60	Experimentally Validated Structures of Supported Metal Nanoclusters on MoS. *Journal of Physical Chemistry Letters*, **2018**, 9, 2972-2978	6.4	13
59	Tuning the hydrogen evolution activity of MoC nanoparticles via control of their growth conditions. *Nanoscale*, **2017**, 9, 3252-3260	7.7	29
58	Effects of Cr-doping on the adsorption and dissociation of S, SO, and SO on Ni(111) surfaces. *Journal of Chemical Physics*, **2017**, 146, 154701	3.9	3
57	Enhanced Mass Transfer in the Step Edge Induced Oxidation on Cu(100) Surface. *Journal of Physical Chemistry C*, **2017**, 121, 11251-11260	3.8	10
56	Role of Surface Stress on the Reactivity of Anatase TiO(001). *Journal of Physical Chemistry Letters*, **2017**, 8, 1764-1771	6.4	29
55	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	16.4	31
54	Structural Stabilities and Electronic Properties of High-Angle Grain Boundaries in Perovskite Cesium Lead Halides. *Journal of Physical Chemistry C*, **2017**, 121, 1715-1722	3.8	80
53	Comparison of Spinel and Monoclinic Crystal Structures of Al2O3 for Simulation of Electron Energy Loss Spectra. *Microscopy and Microanalysis*, **2017**, 23, 2020-2021	0.5	
52	Constructing a Predictive Model of Copper Oxidation from Experiment and Theory. *Microscopy and Microanalysis*, **2017**, 23, 920-921	0.5	3
51	Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface. *Nano Letters*, **2017**, 17, 6435-6442	11.5	120
50	Structures of defects on anatase TiO(001) surfaces. *Nanoscale*, **2017**, 9, 11553-11565	7.7	17
49	Atomically Visualizing Elemental Segregation-Induced Surface Alloying and Restructuring. *Journal of Physical Chemistry Letters*, **2017**, 8, 6035-6040	6.4	9
48	Segregation of Native Defects to the Grain Boundaries in Methylammonium Lead Iodide Perovskite. *Journal of Physical Chemistry Letters*, **2017**, 8, 5935-5942	6.4	40
47	Facile Anhydrous Proton Transport on Hydroxyl Functionalized Graphane. *Physical Review Letters*, **2017**, 118, 186101	7.4	15

46	2D halide perovskite-based van der Waals heterostructures: contact evaluation and performance modulation. *2D Materials*, **2017**, 4, 035009	5.9	18
45	Controlling nucleation, growth, and orientation of metal halide perovskite thin films with rationally selected additives. *Journal of Materials Chemistry A*, **2017**, 5, 113-123	13	92
44	Hydrogen-induced atomic structure evolution of the oxygen-chemisorbed Cu(110) surface. *Journal of Chemical Physics*, **2016**, 145, 234704	3.9	7
43	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	3.8	21
42	Step-Edge Directed Metal Oxidation. *Journal of Physical Chemistry Letters*, **2016**, 7, 2530-6	6.4	18
41	Nano-scale polar-nonpolar oxide heterostructures for photocatalysis. *Nanoscale*, **2016**, 8, 6057-63	7.7	12
40	Temperature Dependence of the Energy Levels of Methylammonium Lead Iodide Perovskite from First-Principles. *Journal of Physical Chemistry Letters*, **2016**, 7, 5247-5252	6.4	69
39	Polarizabilities and van der Waals C6 coefficients of fullerenes from an atomistic electrodynamics model: Anomalous scaling with number of carbon atoms. *Journal of Chemical Physics*, **2016**, 145, 024311	3.9	4
38	Nature of the cubic to tetragonal phase transition in methylammonium lead iodide perovskite. *Journal of Chemical Physics*, **2016**, 145, 144702	3.9	41
37	Early and transient stages of Cu oxidation: Atomistic insights from theoretical simulations and in situ experiments. *Surface Science*, **2016**, 652, 98-113	1.8	26
36	Tunability of the two-dimensional electron gas at the LaAlO/SrTiO interface by strain-induced ferroelectricity. *Physical Chemistry Chemical Physics*, **2016**, 18, 28474-28484	3.6	21
35	Ultrafast Dynamics of Photongenerated Holes at a CHOH/TiO Rutile Interface. *Journal of the American Chemical Society*, **2016**, 138, 13740-13749	16.4	92
34	Temperature dependent energy levels of methylammonium lead iodide perovskite. *Applied Physics Letters*, **2015**, 106, 243904	3.4	133
33	Trends in the Adsorption and Growth Morphology of Metals on the MoS2(001) Surface. *Crystal Growth and Design*, **2015**, 15, 3190-3200	3.5	37
32	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	3.8	26
31	Modified Schottky emission to explain thickness dependence and slow depolarization in BaTiO3 nanowires. *Physical Review B*, **2015**, 91,	3.3	3
30	Investigation of the Structural and Electronic Properties of Pt/Al2O3, a Model Catalyst System. *Microscopy and Microanalysis*, **2015**, 21, 1655-1656	0.5	
29	Step-Induced Oxygen Upward Diffusion on Stepped Cu(100) Surface. *Journal of Physical Chemistry C* , **2015**, 119, 251-261	3.8	16

28	Density Functional Theory Study of Nucleation and Growth of Pt Nanoparticles on MoS2(001) Surface. *Crystal Growth and Design*, **2015**, 15, 642-652	3.5	25
27	Spectroscopic signatures of topological and diatom-vacancy defects in single-walled carbon nanotubes. *Physical Chemistry Chemical Physics*, **2014**, 16, 1479-86	3.6	12
26	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, 7235-41	2.8	8
25	Strong reciprocal interaction between polarization and surface stoichiometry in oxide ferroelectrics. *Nano Letters*, **2014**, 14, 6711-7	11.5	29
24	Role of oxygen in Cu(1 1 0) surface restructuring in the vicinity of step edges. *Chemical Physics Letters*, **2014**, 613, 64-69	2.5	14
23	Surface-step-induced oscillatory oxide growth. *Physical Review Letters*, **2014**, 113, 136104	7.4	44
22	Kinetic Barriers of the Phase Transition in the Oxygen Chemisorbed Cu(110)-(2 □1)-O as a Function of Oxygen Coverage. *Journal of Physical Chemistry C*, **2014**, 118, 20858-20866	3.8	22
21	Van der Waals Epitaxial Growth of Transition Metal Dichalcogenides on Pristine and N-Doped Graphene. *Crystal Growth and Design*, **2014**, 14, 4920-4928	3.5	15
20	Probing single-walled carbon nanotube defect chemistry using resonance Raman spectroscopy. *Carbon*, **2014**, 67, 17-26	10.4	26
19	Insight into the Mechanism of Graphene Oxide Degradation via the Photo-Fenton Reaction. *Journal of Physical Chemistry C*, **2014**, 118, 10519-10529	3.8	85
18	Coexisting surface phases and coherent one-dimensional interfaces on BaTiO3(001). *ACS Nano*, **2014**, 8, 4465-73	16.7	19
17	Oxygen chemisorption-induced surface phase transitions on Cu(110). *Surface Science*, **2014**, 627, 75-84	1.8	30
16	TFOx: A versatile kinetic Monte Carlo program for simulations of island growth in three dimensions. *Computational Materials Science*, **2014**, 91, 292-302	3.2	8
15	Understanding the adsorption of CuPc and ZnPc on noble metal surfaces by combining quantum-mechanical modelling and photoelectron spectroscopy. *Molecules*, **2014**, 19, 2969-92	4.8	66
14	Origins of thermal conductivity changes in strained crystals. *Physical Review B*, **2014**, 90,	3.3	55
13	Influence of strain and metal thickness on metal-MoS□contacts. *Journal of Chemical Physics*, **2014**, 141, 094707	3.9	27
12	Oxygen Reduction Electrocatalysis Using N-Doped Graphene Quantum-Dots. *Journal of Physical Chemistry Letters*, **2013**, 4, 4160-4165	6.4	112
11	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	3.8	82

10	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	3.8	34
9	In situ atomic-scale visualization of oxide islanding during oxidation of Cu surfaces. *Chemical Communications*, **2013**, 49, 10862-4	5.8	43
8	Understanding Structure and Bonding of Multilayered Metal-Organic Nanostructures. *Journal of Physical Chemistry C*, **2013**, 117, 3055-3061	3.8	36
7	The Effect of Metal Catalyst on the Electrocatalytic Activity of Nitrogen-Doped Carbon Nanotubes. *Journal of Physical Chemistry C*, **2013**, 117, 25213-25221	3.8	34
6	Non-additivity of polarizabilities and van der Waals C6 coefficients of fullerenes. *Journal of Chemical Physics*, **2013**, 138, 114107	3.9	29
5	Atomic and Electronic Structure of the BaTiO(3)(001) (sqrt[5] ×sqrt[5])R26.6°Surface Reconstruction. *Physical Review Letters*, **2012**, 109, 256802	7.4	47
4	Ab initio atomistic thermodynamics study of the early stages of Cu(100) oxidation. *Physical Review B*, **2012**, 86,	3.3	35
3	Convergence acceleration in machine learning potentials for atomistic simulations		2
2	Revisiting trends in the exchange current for hydrogen evolution. *Catalysis Science and Technology*,	5.5	4
1	Grain Boundaries in Methylammonium Lead Halide Perovskites Facilitate Water Diffusion. *Advanced Energy and Sustainability Research*,2100087	1.6	2