

Aloysius Soon

List of Publications by Year in descending order

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120
papers

4,772
citations

126708

33
h-index

102304

66
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123
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123
docs citations

123
times ranked

7251
citing authors

#	ARTICLE	IF	CITATIONS
1	Single-Atom Catalyst of Platinum Supported on Titanium Nitride for Selective Electrochemical Reactions. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2058-2062.	7.2	708
2	Support Effects in Single-Atom Platinum Catalysts for Electrochemical Oxygen Reduction. <i>ACS Catalysis</i> , 2017, 7, 1301-1307.	5.5	363
3	Thermodynamic stability and structure of copper oxide surfaces: A first-principles investigation. <i>Physical Review B</i> , 2007, 75, .	1.1	275
4	Oxygen adsorption and stability of surface oxides on Cu(111): A first-principles investigation. <i>Physical Review B</i> , 2006, 73, .	1.1	248
5	Stability and morphology of cerium oxide surfaces in an oxidizing environment: A first-principles investigation. <i>Journal of Chemical Physics</i> , 2009, 131, .	1.2	150
6	Anharmonicity in the High-Temperature C_{2c} Phase of SnSe: Soft Modes and Three-Phonon Interactions. <i>Physical Review Letters</i> , 2016, 117, 075502.	1.1	147
7	Density functional study of oxygen on Cu(100) and Cu(110) surfaces. <i>Physical Review B</i> , 2010, 81, .	1.1	130
8	Shape effects of cuprous oxide particles on stability in water and photocatalytic water splitting. <i>Journal of Materials Chemistry A</i> , 2015, 3, 156-162.	5.2	114
9	Hydrogen-doped viscoplastic liquid metal microparticles for stretchable printed metal lines. <i>Nature Materials</i> , 2021, 20, 533-540.	13.3	111
10	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of Cu_{2-x} . <i>Physical Review B</i> , 2009, 79, .	1.1	109
11	Single-Atom Catalyst of Platinum Supported on Titanium Nitride for Selective Electrochemical Reactions. <i>Angewandte Chemie</i> , 2016, 128, 2098-2102.	1.6	94
12	Influence of Rb/Cs Cation-Exchange on Inorganic Sn Halide Perovskites: From Chemical Structure to Physical Properties. <i>Chemistry of Materials</i> , 2017, 29, 3181-3188.	3.2	89
13	The role of titanium nitride supports for single-atom platinum-based catalysts in fuel cell technology. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16552.	1.3	88
14	Plane-wave pseudopotential density functional theory periodic slab calculations of CO adsorption on Cu ₂ O(111) surface. <i>Surface Science</i> , 2005, 579, 131-140.	0.8	78
15	Steam treatment on Ni ³⁺ -Al ₂ O ₃ for enhanced carbon resistance in combined steam and carbon dioxide reforming of methane. <i>Applied Catalysis B: Environmental</i> , 2013, 134-135, 103-109.	10.8	78
16	The austenite/martensite interface: A first-principles investigation of the fcc Fe(1 1 1)/hcp Fe(0 0 0 1) system. <i>Applied Surface Science</i> , 2012, 258, 9977-9981.	3.1	69
17	Solution-based synthesis of anisotropic metal chalcogenide nanocrystals and their applications. <i>Journal of Materials Chemistry C</i> , 2014, 2, 6222-6248.	2.7	66
18	Electronic structure modification of platinum on titanium nitride resulting in enhanced catalytic activity and durability for oxygen reduction and formic acid oxidation. <i>Applied Catalysis B: Environmental</i> , 2015, 174-175, 35-42.	10.8	63

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19	Surface oxides of the oxygen-copper system: Precursors to the bulk oxide phase?. Surface Science, 2007, 601, 5809-5813.	0.8	60
20	Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111). Physical Review B, 2008, 78, .	1.1	51
21	Identification of critical stacking faults in thin-film CdTe solar cells. Applied Physics Letters, 2014, 105, .	1.5	48
22	Unraveling the Intercalation Chemistry of Hexagonal Tungsten Bronze and Its Optical Responses. Chemistry of Materials, 2016, 28, 4528-4535.	3.2	47
23	Revisiting Polytypism in Hexagonal Ternary Sulfide $ZnIn_2S_4$ for Photocatalytic Hydrogen Production Within the Z-Scheme. Chemistry of Materials, 2019, 31, 9148-9155.	3.2	47
24	Understanding the advantage of hexagonal WO_3 as an efficient photoanode for solar water splitting: a first-principles perspective. Journal of Materials Chemistry A, 2016, 4, 11498-11506.	5.2	45
25	Ab initio lattice dynamics and thermal expansion of Cu_2S . Physical Review B, 2009, 80, 084411.	1.1	43
26	First principles study of 3d transition metal doped Cu_2S . Journal of Magnetism and Magnetic Materials, 2012, 324, 3138-3143.	1.1	40
27	The mechanism of dynamic strain aging for type A serrations in tensile flow curves of Fe-18Mn-0.55C (wt.%) twinning-induced plasticity steel. Acta Materialia, 2020, 188, 366-375.	3.8	40
28	Nitrogen adsorption and thin surface nitrides on Cu(111) from first-principles. Surface Science, 2007, 601, 4775-4785.	0.8	39
29	One-Step Solution Phase Growth of Transition Metal Dichalcogenide Thin Films Directly on Solid Substrates. Advanced Materials, 2017, 29, 1700291.	11.1	39
30	Control over Electron-Phonon Interaction by Dirac Plasmon Engineering in the Bi_2Se_3 Topological Insulator. Nano Letters, 2018, 18, 734-739.	4.5	39
31	Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation. Physical Review B, 2008, 77, .	1.1	38
32	Nonstoichiometric Nucleation and Growth of Multicomponent Nanocrystals in Solution. Accounts of Chemical Research, 2014, 47, 2887-2893.	7.6	38
33	Electronic structure and band alignment of zinc nitride, Zn_3N_2 . RSC Advances, 2014, 4, 3306-3311.	1.7	38
34	Phase Stability Diagrams of Group 6 Magnesium Oxides and Their Implications for Photon-Assisted Applications. Chemistry of Materials, 2019, 31, 4282-4290.	3.2	38
35	Environment-dependent nanomorphology of TiN: the influence of surface vacancies. Nanoscale, 2012, 4, 5183.	2.8	32
36	Exploring stereographic surface energy maps of cubic metals via an effective pair-potential approach. Physical Review B, 2016, 93, .	1.1	32

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37	The Z-phase in 9% Cr ferritic steels: A phase stability analysis. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2009, 505, 1-5.	2.6	31
38	Bismuth Islands for Low-Temperature Sodium-Beta Alumina Batteries. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 2917-2924.	4.0	31
39	Activated chemical bonds in nanoporous and amorphous iridium oxides favor low overpotential for oxygen evolution reaction. <i>Nature Communications</i> , 2022, 13, .	5.8	31
40	A first-principles density functional study of chlorophenol adsorption on Cu ₂ O(110):CuO. <i>Journal of Chemical Physics</i> , 2009, 130, 184505.	1.2	30
41	Playing with Dimensions: Rational Design for Heteroepitaxial n Junctions. <i>Nano Letters</i> , 2012, 12, 68-76.	4.5	29
42	Color of Copper/Copper Oxide. <i>Advanced Materials</i> , 2021, 33, e2007345.	11.1	28
43	Bridging the temperature and pressure gaps: close-packed transition metal surfaces in an oxygen environment. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 184021.	0.7	27
44	Mitigation of CO poisoning on functionalized Pt-TiN surfaces. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19450.	1.3	27
45	Prediction of morphological changes of catalyst materials under reaction conditions by combined ab initio thermodynamics and microkinetic modelling. <i>Catalysis Science and Technology</i> , 2018, 8, 3493-3503.	2.1	27
46	Density Functional Theory Studies of Chloroethene Adsorption on Zerovalent Iron. <i>Environmental Science & Technology</i> , 2009, 43, 1192-1198.	4.6	26
47	Effect of gold subsurface layer on the surface activity and segregation in Pt/Au/Pt ₃ M (where M = Tj ETQq1 1 0.784314 rgBT /Overloc 034707.	1.2	25
48	Synthesis of Atomically Thin Transition Metal Ditelluride Films by Rapid Chemical Transformation in Solution Phase. <i>Chemistry of Materials</i> , 2018, 30, 2463-2473.	3.2	25
49	Why does bromine square palladium off? An ab initio study of brominated palladium and its nanomorphology. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18570-18577.	1.3	24
50	A first-principles study of ultrathin nanofilms of MgO-supported TiN. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2462.	1.3	22
51	Direct observation of grain boundaries in chemical vapor deposited graphene. <i>Carbon</i> , 2017, 115, 147-153.	5.4	22
52	Remarkably low-energy one-dimensional fault line defects in single-layered phosphorene. <i>Nanoscale</i> , 2015, 7, 19073-19079.	2.8	19
53	Assessing the influence of van der Waals corrected exchange-correlation functionals on the anisotropic mechanical properties of coinage metals. <i>Physical Review B</i> , 2016, 94, .	1.1	19
54	Aligning the Band Structures of Polymorphic Molybdenum Oxides and Organic Emitters in Light-Emitting Diodes. <i>Physical Review Applied</i> , 2017, 7, .	1.5	19

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55	Picosecond Competing Dynamics of Apparent Semiconducting-Metallic Phase Transition in the Topological Insulator Bi_2Se_3 . ACS Photonics, 2020, 7, 759-764.	3.2	19
56	In Situ Defect Engineering Route to Optimize the Cationic Redox Activity of Layered Double Hydroxide Nanosheet via Strong Electronic Coupling with Holey Substrate. Advanced Science, 2022, 9, e2103368.	5.6	19
57	Carbon monoxide reaction with $\text{UO}_2(111)$ single crystal surfaces: A theoretical and experimental study. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2005, 23, 1078-1084.	0.9	18
58	Comparison of hydrogen and deuterium adsorption on $\text{Pd}(100)$. Journal of Chemical Physics, 2010, 132, 024714.	1.2	18
59	Re-visiting the $\text{O}/\text{Cu}(111)$ system “when metastable surface oxides could become an issue!. Physical Chemistry Chemical Physics, 2014, 16, 26735-26740.	1.3	18
60	Synthesis of surfactant-free SnS nanoplates in an aqueous solution. RSC Advances, 2015, 5, 94796-94801.	1.7	18
61	Ab-initio Study of Interactions of Gold Atoms with Hydroxylated $\text{MgO}(001)$ Surfaces. Journal of the Physical Society of Japan, 2012, 81, 054601.	0.7	17
62	Adsorption and Surface Diffusion of Pt Atoms on Hydroxylated $\text{MgO}(001)$ Surfaces. Journal of the Physical Society of Japan, 2013, 82, 034603.	0.7	16
63	Remarkably stable amorphous metal oxide grown on Zr-Cu-Be metallic glass. Scientific Reports, 2015, 5, 18196.	1.6	16
64	Designing Two-Dimensional Dirac Heterointerfaces of Few-Layer Graphene and Tetradymite-Type Sb_2Te_3 for Thermoelectric Applications. ACS Applied Materials & Interfaces, 2017, 9, 42050-42057.	4.0	14
65	Disentangling the Effects of Inter- and Intra-octahedral Distortions on the Electronic Structure in Binary Metal Trioxides. Journal of Physical Chemistry C, 2018, 122, 3558-3566.	1.5	14
66	Examining the rudimentary steps of the oxygen reduction reaction on single-atomic Pt using Ti-based non-oxide supports. Journal of Industrial and Engineering Chemistry, 2018, 58, 208-215.	2.9	14
67	Growing Ultrathin Cu_2O Films on Highly Crystalline $\text{Cu}(111)$: A Closer Inspection from Microscopy and Theory. Journal of Physical Chemistry C, 2019, 123, 12716-12721.	1.5	14
68	Polar oxide substrates for graphene growth: A first-principles investigation of graphene on $\text{MgO}(111)$. Current Applied Physics, 2013, 13, 803-807.	1.1	13
69	Novel polymorphic phase of two-dimensional VSe_2 : the $1T'$ structure and its lattice dynamics. Nanoscale, 2019, 11, 20096-20101.	2.8	13
70	Solid-state chemistry of glassy antimony oxides. Journal of Materials Chemistry C, 2015, 3, 11349-11356.	2.7	12
71	Unraveling the origins of conduction band valley degeneracies in $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$ thermoelectrics. Physical Chemistry Chemical Physics, 2016, 18, 939-946.	1.3	12
72	Experimental Demonstration of in Situ Stress-Driven Optical Modulations in Flexible Semiconducting Thin Films with Enhanced Photodetecting Capability. Chemistry of Materials, 2018, 30, 7776-7781.	3.2	12

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73	Completing the picture of initial oxidation on copper. <i>Applied Surface Science</i> , 2021, 562, 150148.	3.1	12
74	<i>Ab Initio</i> Thermodynamics of Surface Oxide Structures under Controlled Growth Conditions. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2228-2233.	1.5	11
75	Origin of Prestress-Driven Optical Modulations of Flexible ZnO Thin Films Processed in Stretching Mode. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5934-5939.	2.1	11
76	Using Feature-Assisted Machine Learning Algorithms to Boost Polarity in Lead-Free Multicomponent Niobate Alloys for High-Performance Ferroelectrics. <i>Advanced Science</i> , 2022, 9, e2104569.	5.6	11
77	Eventual Chemical Transformation of Metals and Chalcogens into Metal Chalcogenide Nanoplates through a Surface Nucleation-Detachment-Reorganization Mechanism. <i>Chemistry of Materials</i> , 2017, 29, 3219-3227.	3.2	10
78	Anisotropic vacancy-mediated phonon mode softening in Sm and Gd doped ceria. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10048-10059.	1.3	10
79	Atomic order, electronic structure and thermodynamic stability of nickel aluminate. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25952-25961.	1.3	10
80	Thermally Induced Desulfurization: Structural Transformation of Thiophene on the Si(100) Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11731-11737.	1.5	9
81	Adsorption of 2-chlorophenol on Cu ₂ O(111) – CuCUS: A first-principles density functional study. <i>Applied Surface Science</i> , 2010, 256, 4764-4770.	3.1	8
82	First-principles based phenomenological study of Ni nanocubes: The effects of nanostructuring on carbon poisoning of Ni(001) nanofacets. <i>Applied Surface Science</i> , 2013, 265, 339-345.	3.1	8
83	Stacking-dependent energetics and electronic structure of ultrathin polymorphic V_2VI_3 topological insulator nanofilms. <i>Physical Review B</i> , 2014, 90, .	1.1	8
84	The effect of Se doping on the growth of Te nanorods. <i>CrystEngComm</i> , 2015, 17, 5734-5743.	1.3	8
85	Acute mechano-electronic responses in twisted phosphorene nanoribbons. <i>Nanoscale</i> , 2016, 8, 14778-14784.	2.8	8
86	Polymorphic expressions of ultrathin oxidic layers of Mo on Au(111). <i>Nanoscale</i> , 2019, 11, 6023-6035.	2.8	8
87	Atomic Structure and Work Function Modulations in Two-Dimensional Ultrathin CuI Films on Cu(111) from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 16362-16370.	1.5	8
88	Size and dimension effect on volume plasmon energy of nanomaterials. <i>Solid State Communications</i> , 2012, 152, 1564-1566.	0.9	7
89	Interfacial properties in ultrathin MgO films on TiN(001) surfaces: Ab-initio calculations. <i>Journal of the Korean Physical Society</i> , 2014, 64, 289-294.	0.3	7
90	Lattice-mismatched heteroepitaxy of IV-VI thin films on PbTe(001): An ab initio study. <i>Physical Review B</i> , 2015, 91, .	1.1	7

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91	In search of non-conventional surface oxidic motifs of Cu on Au(111). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7349-7358.	1.3	7
92	Polytypism in Hexagonal Tungsten Trioxide: Insights from Ab Initio Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21644-21650.	1.5	7
93	Effect of phonon confinement on the thermal conductivity of In _{0.53} Ga _{0.47} As nanofilms. <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	7
94	Revisiting the Role of the Triple-Phase Boundary in Promoting the Oxygen Reduction Reaction in Aluminum-Air Batteries. <i>Advanced Functional Materials</i> , 2021, 31, 2101720.	7.8	7
95	Composition-controlled ultrathin holey TiO _{2-x} N _x nanosheets as powerful hybridization matrices for highly mass-efficient electrocatalysts. <i>Chemical Engineering Journal</i> , 2022, 437, 135415.	6.6	7
96	Explicating the irreversible electric-field-assisted ferroelectric phase transition in the otherwise antiferroelectric sodium niobate for energy storage systems. <i>Journal of Materials Chemistry C</i> , 2022, 10, 10500-10510.	2.7	7
97	Early transition metal dopants in cuprous oxide: To spin or not to spin. <i>Current Applied Physics</i> , 2013, 13, 1707-1712.	1.1	6
98	A rational computational study of surface defect-mediated stabilization of low-dimensional Pt nanostructures on TiN(100). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9680-9686.	1.3	6
99	Organics on oxidic metal surfaces: a first-principles DFT study of PMDA and ODA fragments on the pristine and mildly oxidized surfaces of Cu(111). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21893-21902.	1.3	6
100	Chemically Driven Enhancement of Oxygen Reduction Electrocatalysis in Supported Perovskite Oxides. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 235-242.	2.1	6
101	Over-Stoichiometry in Heavy Metal Oxides: The Case of Iono-Covalent Tantalum Trioxides. <i>Inorganic Chemistry</i> , 2018, 57, 6057-6064.	1.9	6
102	Understanding the Enhancement of Ionic Transport in Heterogeneously Doped Zirconia by Heterointerface Engineering. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22374-22388.	1.5	5
103	Enhanced polarization in epitaxially strained monoclinic potassium niobate for lead-free electromechanical applications. <i>Journal of Materials Chemistry C</i> , 2021, 9, 13420-13431.	2.7	5
104	Direct observation of trapped charges at ReSe ₂ and graphene heterojunctions. <i>Applied Surface Science</i> , 2022, 579, 152187.	3.1	5
105	In-plane optical and electrical anisotropy in low-symmetry layered GeS microribbons. <i>NPG Asia Materials</i> , 2022, 14, .	3.8	5
106	A computational survey of metal-free polyimide-based photocatalysts within the single-stranded polymer model. <i>Molecular Catalysis</i> , 2020, 497, 111184.	1.0	4
107	Aluminium adsorption on Ir(111) at a quarter monolayer coverage: A first-principles study. <i>Applied Surface Science</i> , 2008, 254, 7655-7658.	3.1	3
108	Uncovering the Thermo-Kinetic Origins of Phase Ordering in Mixed-Valence Antimony Tetroxide by First-Principles Modeling. <i>Inorganic Chemistry</i> , 2017, 56, 6545-6550.	1.9	3

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109	Non-dissociative adsorption of glycerol on the (111) surface of Ni and Pt-based metallic systems: Hints on reforming activity from d-band center. <i>Molecular Catalysis</i> , 2019, 474, 110412.	1.0	3
110	Tunable Threshold Voltage of ZnTe-Based Ovonic Switching Devices via Isovalent Cation Exchange. <i>ACS Applied Electronic Materials</i> , 2021, 3, 1107-1114.	2.0	3
111	First-Principles Calculations of Heteroanionic Monochalcogenide Alloy Nanosheets with Direction-dependent Properties for Anisotropic Optoelectronics. <i>ACS Applied Nano Materials</i> , 2021, 4, 5912-5920.	2.4	3
112	Ab Initio Surface Phase Diagram of Sn/Cu(001) : Reconciling Experiments with Theory. <i>Physical Review Applied</i> , 2017, 8, .	1.5	2
113	Stretching-Driven Crystal Anisotropy and Optical Modulations of Flexible Wide Band Gap Inorganic Thin Films. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 41516-41522.	4.0	2
114	Alternative Cu ₃ Zn catalysts for enhanced reduction of CO ₂ to CH ₄ : A density functional theory-based approach. <i>Surfaces and Interfaces</i> , 2022, 31, 102030.	1.5	2
115	Publisher's Note: Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation [Phys. Rev. B 77, 125423 (2008)]. <i>Physical Review B</i> , 2008, 77, .	1.1	1
116	Assembling phosphorene flexagons for 2D electron-density-guided nanopatterning and nanofabrication. <i>Nanoscale</i> , 2017, 9, 10465-10474.	2.8	1
117	Going beyond the equilibrium crystal shape: re-tracing the morphological evolution in group 5 tetradymite nanocrystals. <i>Nanoscale</i> , 2021, 13, 15721-15730.	2.8	0
118	Defect-mediated ab initio thermodynamics of metastable $\hat{\Gamma}^3$ -MoN(001). <i>Journal of Chemical Physics</i> , 2021, 154, 064703.	1.2	0
119	Controlling electron-phonon interaction in the Bi ₂ Se ₃ topological insulator by Dirac-plasmon engineering. , 2018, , .		0
120	Electric Control over 2D Dirac Plasmon Resonances in Topological Insulator Bi ₂ Se ₃ in Proximity Contact with Graphene. , 2019, , .		0