Aloysius Soon

List of Publications by Year
in descending order

120 papers	4,772 citations	126708 33 h-index	102304 66 g-index
123 all docs	123 docs citations	123 times ranked	7251 citing authors

#	Article	IF	Citations
1	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
2	Direct observation of trapped charges at ReSe2 and graphene heterojunctions. Applied Surface Science, 2022, 579, 152187.	3.1	5
3	Using Featureâ€Assisted Machine Learning Algorithms to Boost Polarity in Leadâ€Free Multicomponent Niobate Alloys for Highâ€Performance Ferroelectrics. Advanced Science, 2022, 9, e2104569.	5.6	11
4	Composition-controlled ultrathin holey TiO1âˆ’xNx nanosheets as powerful hybridization matrices for highly mass-efficient electrocatalysts. Chemical Engineering Journal, 2022, 437, 135415.	6.6	7
5	In-plane optical and electrical anisotropy in low-symmetry layered GeS microribbons. NPG Asia Materials, 2022, 14, .	3.8	5
6	Alternative Cu3Zn catalysts for enhanced reduction of CO2 to CH4: A density functional theory-based approach. Surfaces and Interfaces, 2022, 31, 102030.	1.5	2
7	Activated chemical bonds in nanoporous and amorphous iridium oxides favor low overpotential for oxygen evolution reaction. Nature Communications, 2022, 13, .	5.8	31
8	Explicating the irreversible electric-field-assisted ferroelectric phase transition in the otherwise antiferroelectric sodium niobate for energy storage systems. Journal of Materials Chemistry C, 2022, 10, 10500-10510.	2.7	7
9	Going beyond the equilibrium crystal shape: re-tracing the morphological evolution in group 5 tetradymite nanocrystals. Nanoscale, 2021, 13, 15721-15730.	2.8	0
10	Hydrogen-doped viscoplastic liquid metal microparticles for stretchable printed metal lines. Nature Materials, 2021, 20, 533-540.	13.3	111
11	Enhanced polarization in epitaxially strained monoclinic potassium niobate for lead-free electromechanical applications. Journal of Materials Chemistry C, 2021, 9, 13420-13431.	2.7	5
12	Tunable Threshold Voltage of ZnTe-Based Ovonic Switching Devices via Isovalent Cation Exchange. ACS Applied Electronic Materials, 2021, 3, 1107-1114.	2.0	3
13	Defect-mediated ab initio thermodynamics of metastable Î³-MoN(001). Journal of Chemical Physics, 2021, 154, 064703.	1.2	0
14	Color of Copper/Copper Oxide. Advanced Materials, 2021, 33, e2007345.	11.1	28
15	First-Principles Calculations of Heteroanionic Monochalcogenide Alloy Nanosheets with Direction-dependent Properties for Anisotropic Optoelectronics. ACS Applied Nano Materials, 2021, 4, 5912-5920.	2.4	3
16	Revisiting the Role of the Tripleâ€Phase Boundary in Promoting the Oxygen Reduction Reaction in Aluminumâ€“Air Batteries. Advanced Functional Materials, 2021, 31, 2101720.	7.8	7
17	Completing the picture of initial oxidation on copper. Applied Surface Science, 2021, 562, 150148.	3.1	12
18	Picosecond Competing Dynamics of Apparent Semiconducting-Metallic Phase Transition in the Topological Insulator Bi₂Se₃. ACS Photonics, 2020, 7, 759-764.	3.2	19

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19	Atomic Structure and Work Function Modulations in Two-Dimensional Ultrathin CuI Films on Cu(111) from First-Principles Calculations. Journal of Physical Chemistry C, 2020, 124, 16362-16370.	1.5	8
20	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
21	A computational survey of metal-free polyimide-based photocatalysts within the single-stranded polymer model. Molecular Catalysis, 2020, 497, 111184.	1.0	4
22	Stretching-Driven Crystal Anisotropy and Optical Modulations of Flexible Wide Band Gap Inorganic Thin Films. ACS Applied Materials & Interfaces, 2019, 11, 41516-41522.	4.0	2
23	Revisiting Polytypism in Hexagonal Ternary Sulfide ZnIn₂S₄ for Photocatalytic Hydrogen Production Within the Z-Scheme. Chemistry of Materials, 2019, 31, 9148-9155.	3.2	47
24	Non-dissociative adsorption of glycerol on the (111) surface of Ni and Pt-based metallic systems: Hints on reforming activity from d-band center. Molecular Catalysis, 2019, 474, 110412.	1.0	3
25	Phase Stability Diagrams of Group 6 MagnÃ©li Oxides and Their Implications for Photon-Assisted Applications. Chemistry of Materials, 2019, 31, 4282-4290.	3.2	38
26	Growing Ultrathin Cu₂O Films on Highly Crystalline Cu(111): A Closer Inspection from Microscopy and Theory. Journal of Physical Chemistry C, 2019, 123, 12716-12721.	1.5	14
27	Polymorphic expressions of ultrathin oxidic layers of Mo on Au(111). Nanoscale, 2019, 11, 6023-6035.	2.8	8
28	Novel polymorphic phase of two-dimensional VSe₂: the 1Tâ€² structure and its lattice dynamics. Nanoscale, 2019, 11, 20096-20101.	2.8	13
29	Atomic order, electronic structure and thermodynamic stability of nickel aluminate. Physical Chemistry Chemical Physics, 2019, 21, 25952-25961.	1.3	10
30	Bismuth Islands for Low-Temperature Sodium-Beta Alumina Batteries. ACS Applied Materials & Interfaces, 2019, 11, 2917-2924.	4.0	31
31	Electric Control over 2D Dirac Plasmon Resonances in Topological Insulator Bi2Se3 in Proximity Contact with Graphene. , 2019, , .		0
32	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
33	Control over Electronâ€“Phonon Interaction by Dirac Plasmon Engineering in the Bi₂Se₃ Topological Insulator. Nano Letters, 2018, 18, 734-739.	4.5	39
34	Over-Stoichiometry in Heavy Metal Oxides: The Case of Iono-Covalent Tantalum Trioxides. Inorganic Chemistry, 2018, 57, 6057-6064.	1.9	6
35	Synthesis of Atomically Thin Transition Metal Ditelluride Films by Rapid Chemical Transformation in Solution Phase. Chemistry of Materials, 2018, 30, 2463-2473.	3.2	25
36	Anisotropic vacancy-mediated phonon mode softening in Sm and Gd doped ceria. Physical Chemistry Chemical Physics, 2018, 20, 10048-10059.	1.3	10

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37	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
38	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
39	Origin of Prestress-Driven Optical Modulations of Flexible ZnO Thin Films Processed in Stretching Mode. Journal of Physical Chemistry Letters, 2018, 9, 5934-5939.	2.1	11
40	Understanding the Enhancement of Ionic Transport in Heterogeneously Doped Zirconia by Heterointerface Engineering. Journal of Physical Chemistry C, 2018, 122, 22374-22388.	1.5	5
41	Polytypism in Hexagonal Tungsten Trioxide: Insights from Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 21644-21650.	1.5	7
42	Prediction of morphological changes of catalyst materials under reaction conditions by combined ab initio thermodynamics and microkinetic modelling. Catalysis Science and Technology, 2018, 8, 3493-3503.	2.1	27
43	Effect of phonon confinement on the thermal conductivity of In0.53Ga0.47As nanofilms. Journal of Applied Physics, 2018, 123, .	1.1	7
44	Controlling electron-phonon interaction in the Bi2Se3 topological insulator by Dirac-plasmon engineering. , 2018, , .		0
45	Ab Initio Thermodynamics of Surface Oxide Structures under Controlled Growth Conditions. Journal of Physical Chemistry C, 2017, 121, 2228-2233.	1.5	11
46	Direct observation of grain boundaries in chemical vapor deposited graphene. Carbon, 2017, 115, 147-153.	5.4	22
47	Aligning the Band Structures of Polymorphic Molybdenum Oxides and Organic Emitters in Light-Emitting Diodes. Physical Review Applied, 2017, 7, .	1.5	19
48	Oneâ€Step Solution Phase Growth of Transition Metal Dichalcogenide Thin Films Directly on Solid Substrates. Advanced Materials, 2017, 29, 1700291.	11.1	39
49	Uncovering the Thermo-Kinetic Origins of Phase Ordering in Mixed-Valence Antimony Tetroxide by First-Principles Modeling. Inorganic Chemistry, 2017, 56, 6545-6550.	1.9	3
50	Influence of Rb/Cs Cation-Exchange on Inorganic Sn Halide Perovskites: From Chemical Structure to Physical Properties. Chemistry of Materials, 2017, 29, 3181-3188.	3.2	89
51	Eventual Chemical Transformation of Metals and Chalcogens into Metal Chalcogenide Nanoplates through a Surface Nucleation-Detachment-Reorganization Mechanism. Chemistry of Materials, 2017, 29, 3219-3227.	3.2	10
52	Support Effects in Single-Atom Platinum Catalysts for Electrochemical Oxygen Reduction. ACS Catalysis, 2017, 7, 1301-1307.	5.5	363
53	Chemically Driven Enhancement of Oxygen Reduction Electrocatalysis in Supported Perovskite Oxides. Journal of Physical Chemistry Letters, 2017, 8, 235-242.	2.1	6
54	AbÂinitio Surface Phase Diagram of Sn/Cu(001) : Reconciling Experiments with Theory. Physical Review Applied, 2017, 8, .	1.5	2

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55	Assembling phosphorene flexagons for 2D electron-density-guided nanopatterning and nanofabrication. Nanoscale, 2017, 9, 10465-10474.	2.8	1
56	Designing Two-Dimensional Dirac Heterointerfaces of Few-Layer Graphene and Tetradymite-Type Sb₂Te₃ for Thermoelectric Applications. ACS Applied Materials & Interfaces, 2017, 9, 42050-42057.	4.0	14
57	Acute mechano-electronic responses in twisted phosphorene nanoribbons. Nanoscale, 2016, 8, 14778-14784.	2.8	8
58	Anharmonicity in the High-Temperature<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>C</mml:mi><mml:mi>m</mml:mi><mml:mi>c</mml:mi><mml:mi>m</mml:mi></mml:math>Phase of SnSe: Soft Modes and Three-Phonon Interactions. Physical Review Letters, 2016, 117, 075502.	2.8	247
59	Exploring stereographic surface energy maps of cubic metals via an effective pair-potential approach. Physical Review B, 2016, 93, .	1.1	32
60	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). Physical Chemistry Chemical Physics, 2016, 18, 21893-21902.	1.3	6
61	Assessing the influence of van der Waals corrected exchange-correlation functionals on the anisotropic mechanical properties of coinage metals. Physical Review B, 2016, 94, .	1.1	19
62	Singleâ€Atom Catalyst of Platinum Supported on Titanium Nitride for Selective Electrochemical Reactions. Angewandte Chemie, 2016, 128, 2098-2102.	1.6	94
63	Singleâ€Atom Catalyst of Platinum Supported on Titanium Nitride for Selective Electrochemical Reactions. Angewandte Chemie - International Edition, 2016, 55, 2058-2062.	7.2	708
64	Understanding the advantage of hexagonal WO₃as an efficient photoanode for solar water splitting: a first-principles perspective. Journal of Materials Chemistry A, 2016, 4, 11498-11506.	5.2	45
65	Unraveling the Intercalation Chemistry of Hexagonal Tungsten Bronze and Its Optical Responses. Chemistry of Materials, 2016, 28, 4528-4535.	3.2	47
66	Unraveling the origins of conduction band valley degeneracies in Mg2Si1â^'xSnx thermoelectrics. Physical Chemistry Chemical Physics, 2016, 18, 939-946.	1.3	12
67	In search of non-conventional surface oxidic motifs of Cu on Au(111). Physical Chemistry Chemical Physics, 2016, 18, 7349-7358.	1.3	7
68	Remarkably stable amorphous metal oxide grown on Zr-Cu-Be metallic glass. Scientific Reports, 2015, 5, 18196.	1.6	16
69	Electronic structure modification of platinum on titanium nitride resulting in enhanced catalytic activity and durability for oxygen reduction and formic acid oxidation. Applied Catalysis B: Environmental, 2015, 174-175, 35-42.	10.8	63
70	A rational computational study of surface defect-mediated stabilization of low-dimensional Pt nanostructures on TiN(100). Physical Chemistry Chemical Physics, 2015, 17, 9680-9686.	1.3	6
71	Synthesis of surfactant-free SnS nanoplates in an aqueous solution. RSC Advances, 2015, 5, 94796-94801.	1.7	18
72	Remarkably low-energy one-dimensional fault line defects in single-layered phosphorene. Nanoscale, 2015, 7, 19073-19079.	2.8	19

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73	Effect of gold subsurface layer on the surface activity and segregation in Pt/Au/Pt3M (where M =) Tj ETQq1 1 0.784314 rgBT /Overloc 034707.	1.2	25
74	Lattice-mismatched heteroepitaxy of IV-VI thin films on PbTe(001): Anab initiostudy. Physical Review B, 2015, 91, .	1.1	7
75	The effect of Se doping on the growth of Te nanorods. CrystEngComm, 2015, 17, 5734-5743.	1.3	8
76	Solid-state chemistry of glassy antimony oxides. Journal of Materials Chemistry C, 2015, 3, 11349-11356.	2.7	12
77	Shape effects of cuprous oxide particles on stability in water and photocatalytic water splitting. Journal of Materials Chemistry A, 2015, 3, 156-162.	5.2	114
78	Stacking-dependent energetics and electronic structure of ultrathin polymorphic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">VI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>topological insulator nanofilms. Physical Review B, 2014, 90, .	1.1	8
79	Identification of critical stacking faults in thin-film CdTe solar cells. Applied Physics Letters, 2014, 105, .	1.5	48
80	Interfacial properties in ultrathin MgO films on TiN(001) surfaces: Ab-initio calculations. Journal of the Korean Physical Society, 2014, 64, 289-294.	0.3	7
81	Why does bromine square palladium off? An ab initio study of brominated palladium and its nanomorphology. Physical Chemistry Chemical Physics, 2014, 16, 18570-18577.	1.3	24
82	Nonstoichiometric Nucleation and Growth of Multicomponent Nanocrystals in Solution. Accounts of Chemical Research, 2014, 47, 2887-2893.	7.6	38
83	Electronic structure and band alignment of zinc nitride, Zn₃N₂. RSC Advances, 2014, 4, 3306-3311.	1.7	38
84	Re-visiting the O/Cu(111) system â€“ when metastable surface oxides could become an issue!. Physical Chemistry Chemical Physics, 2014, 16, 26735-26740.	1.3	18
85	Solution-based synthesis of anisotropic metal chalcogenide nanocrystals and their applications. Journal of Materials Chemistry C, 2014, 2, 6222-6248.	2.7	66
86	Steam treatment on Ni/Î³-Al2O3 for enhanced carbon resistance in combined steam and carbon dioxide reforming of methane. Applied Catalysis B: Environmental, 2013, 134-135, 103-109.	10.8	78
87	Polar oxide substrates for graphene growth: A first-principles investigation of graphene on MgO(111). Current Applied Physics, 2013, 13, 803-807.	1.1	13
88	Mitigation of CO poisoning on functionalized Ptâ€“TiN surfaces. Physical Chemistry Chemical Physics, 2013, 15, 19450.	1.3	27
89	First-principles based phenomenological study of Ni nanocubes: The effects of nanostructuring on carbon poisoning of Ni(0 0 1) nanofacets. Applied Surface Science, 2013, 265, 339-345.	3.1	8
90	Early transition metal dopants in cuprous oxide: To spin or not to spin. Current Applied Physics, 2013, 13, 1707-1712.	1.1	6

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91	Thermally Induced Desulfurization: Structural Transformation of Thiophene on the Si(100) Surface. Journal of Physical Chemistry C, 2013, 117, 11731-11737.	1.5	9
92	Adsorption and Surface Diffusion of Pt Atoms on Hydroxylated MgO(001) Surfaces. Journal of the Physical Society of Japan, 2013, 82, 034603.	0.7	16
93	Ab-initio Study of Interactions of Gold Atoms with Hydroxylated MgO(001) Surfaces. Journal of the Physical Society of Japan, 2012, 81, 054601.	0.7	17
94	Environment-dependent nanomorphology of TiN: the influence of surface vacancies. Nanoscale, 2012, 4, 5183.	2.8	32
95	Size and dimension effect on volume plasmon energy of nanomaterials. Solid State Communications, 2012, 152, 1564-1566.	0.9	7
96	Playing with Dimensions: Rational Design for Heteroepitaxial pâ€“n Junctions. Nano Letters, 2012, 12, 68-76.	4.5	29
97	The austenite/É› martensite interface: A first-principles investigation of the fcc Fe(1 1 1)/hcp Fe(0 0 0 1) system. Applied Surface Science, 2012, 258, 9977-9981.	3.1	69
98	First principles study of 3d transition metal doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0020.gif" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Cu</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>. Journal of Magnetism and Magnetic Materials, 2012, 324, 3138-3143.	1.0	40
99	The role of titanium nitride supports for single-atom platinum-based catalysts in fuel cell technology. Physical Chemistry Chemical Physics, 2012, 14, 16552.	1.3	88
100	A first-principles study of ultrathin nanofilms of MgO-supported TiN. Physical Chemistry Chemical Physics, 2012, 14, 2462.	1.3	22
101	Adsorption of 2-chlorophenol on Cu2O(111)â€“CuCUS: A first-principles density functional study. Applied Surface Science, 2010, 256, 4764-4770.	3.1	8
102	Comparison of hydrogen and deuterium adsorption on Pd(100). Journal of Chemical Physics, 2010, 132, 024714.	1.2	18
103	Density functional study of oxygen on Cu(100) and Cu(110) surfaces. Physical Review B, 2010, 81, .	1.1	130
104	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 79, .	1.1	109
105	A first-principles density functional study of chlorophenol adsorption on Cu2O(110):CuO. Journal of Chemical Physics, 2009, 130, 184505.	1.2	30
106	The Z-phase in 9â€“12% Cr ferritic steels: A phase stability analysis. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2009, 505, 1-5.	2.6	31
107	Ab initiolattice dynamics and thermal expansion of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 80, .	1.1	43
108	Density Functional Theory Studies of Chloroethene Adsorption on Zerovalent Iron. Environmental Science & Technology, 2009, 43, 1192-1198.	4.6	26

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109	Stability and morphology of cerium oxide surfaces in an oxidizing environment: A first-principles investigation. Journal of Chemical Physics, 2009, 131, .	1.2	150
110	Aluminium adsorption on Ir(111) at a quarter monolayer coverage: A first-principles study. Applied Surface Science, 2008, 254, 7655-7658.	3.1	3
111	Bridging the temperature and pressure gaps: close-packed transition metal surfaces in an oxygen environment. Journal of Physics Condensed Matter, 2008, 20, 184021.	0.7	27
112	Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation. Physical Review B, 2008, 77, .	1.1	38
113	Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111). Physical Review B, 2008, 78, .	1.1	51
114	Publisher's Note: Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation [Phys. Rev. B77, 125423 (2008)]. Physical Review B, 2008, 77, .	1.1	1
115	Thermodynamic stability and structure of copper oxide surfaces: A first-principles investigation. Physical Review B, 2007, 75, .	1.1	275
116	Nitrogen adsorption and thin surface nitrides on Cu(111) from first-principles. Surface Science, 2007, 601, 4775-4785.	0.8	39
117	Surface oxides of the oxygenâ€“copper system: Precursors to the bulk oxide phase?. Surface Science, 2007, 601, 5809-5813.	0.8	60
118	Oxygen adsorption and stability of surface oxides onCu(111): A first-principles investigation. Physical Review B, 2006, 73, .	1.1	248
119	Plane-wave pseudopotential density functional theory periodic slab calculations of CO adsorption on Cu2O(111) surface. Surface Science, 2005, 579, 131-140.	0.8	78
120	Carbon monoxide reaction with UO2(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