Michael Nolan

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4897010/publications.pdf

Version: 2024-02-01

168 papers	7,650 citations	53660 45 h-index	58464 82 g-index
244 all docs	244 docs citations	244 times ranked	8724 citing authors

#	Article	IF	Citations
1	The electronic structure of oxygen vacancy defects at the low index surfaces of ceria. Surface Science, 2005, 595, 223-232.	0.8	690
2	Density functional theory studies of the structure and electronic structure of pure and defective low index surfaces of ceria. Surface Science, 2005, 576, 217-229.	0.8	683
3	The p-type conduction mechanism in Cu2O: a first principles study. Physical Chemistry Chemical Physics, 2006, 8, 5350.	1.3	307
4	Oxygen vacancy formation and migration in ceria. Solid State Ionics, 2006, 177, 3069-3074.	1.3	290
5	Silicon Nanowire Band Gap Modification. Nano Letters, 2007, 7, 34-38.	4.5	215
6	The Surface Dependence of CO Adsorption on Ceria. Journal of Physical Chemistry B, 2006, 110, 16600-16606.	1.2	172
7	Enhanced oxygen vacancy formation in ceria (111) and (110) surfaces doped with divalent cations. Journal of Materials Chemistry, 2011, 21, 9160.	6.7	153
8	Reduction mechanisms of the CuO(111) surface through surface oxygen vacancy formation and hydrogen adsorption. Physical Chemistry Chemical Physics, 2014, 16, 3036.	1.3	153
9	Cu-Doped TiO2: Visible Light Assisted Photocatalytic Antimicrobial Activity. Applied Sciences (Switzerland), 2018, 8, 2067.	1.3	149
10	Design of Novel Visible Light Active Photocatalyst Materials: Surface Modified TiO₂. Advanced Materials, 2016, 28, 5425-5446.	11.1	144
11	Electronic structure of point defects in controlled self-doping of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> surface: Combined photoemission spectroscopy and density functional theory study. Physical Review B, 2008, 77, .	1.1	138
12	Vacancy formation and CO adsorption on gold-doped ceria surfaces. Surface Science, 2008, 602, 2734-2742.	0.8	125
13	Key scientific challenges in current rechargeable non-aqueous Liâ€“O2 batteries: experiment and theory. Physical Chemistry Chemical Physics, 2014, 16, 12093.	1.3	120
14	Inâ€…Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metalâ€“Support Interactions and Câ^'H Bond Activation at Low Temperature. Angewandte Chemie - International Edition, 2017, 56, 13041-13046.	7.2	120
15	Effect of Cu doping on the anatase-to-rutile phase transition in TiO2 photocatalysts: Theory and experiments. Applied Catalysis B: Environmental, 2019, 246, 266-276.	10.8	119
16	Reduction of NO2on Ceria Surfaces. Journal of Physical Chemistry B, 2006, 110, 2256-2262.	1.2	117
17	Hole localization in Al doped silica: A DFT+U description. Journal of Chemical Physics, 2006, 125, 144701.	1.2	113
18	Spinel-Structured ZnCr₂O₄ with Excess Zn Is the Active ZnO/Cr₂O₃ Catalyst for High-Temperature Methanol Synthesis. ACS Catalysis, 2017, 7, 7610-7622.	5.5	109

#	Article	IF	Citations
19	CeO2catalysed conversion of CO, NO2and NO from first principles energetics. Physical Chemistry Chemical Physics, 2006, 8, 216-218.	1.3	107
20	Surface Sensitivity in Lithium-Doping of MgO:â€‰ A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. Journal of Physical Chemistry C, 2007, 111, 7971-7979.	1.5	96
21	Charge Compensation and Ce³⁺Formation in Trivalent Doping of the CeO₂(110) Surface: The Key Role of Dopant Ionic Radius. Journal of Physical Chemistry C, 2011, 115, 6671-6681.	1.5	95
22	Molecular Adsorption on the Doped (110) Ceria Surface. Journal of Physical Chemistry C, 2009, 113, 2425-2432.	1.5	92
23	Interactions between Thiol Molecular Linkers and the Au13Nanoparticle. Journal of Physical Chemistry B, 2002, 106, 5931-5937.	1.2	80
24	Molecular-Scale Transition Metal Oxide Nanocluster Surface-Modified Titanium Dioxide as Solar-Activated Environmental Catalysts. Journal of Physical Chemistry C, 2014, 118, 12077-12086.	1.5	80
25	Electronic Structure and Reactivity of Ce- and Zr-Doped TiO₂: Assessing the Reliability of Density Functional Theory Approaches. Journal of Physical Chemistry C, 2011, 115, 12995-13007.	1.5	78
26	Hybrid density functional theory description of oxygen vacancies in the CeO2 (110) and (100) surfaces. Chemical Physics Letters, 2010, 499, 126-130.	1.2	71
27	Indium-Doped TiO₂ Photocatalysts with High-Temperature Anatase Stability. Journal of Physical Chemistry C, 2019, 123, 21083-21096.	1.5	69
28	Origin of the Visible-Light Response of Nickel(II) Oxide Cluster Surface Modified Titanium(IV) Dioxide. Journal of Physical Chemistry C, 2013, 117, 2709-2718.	1.5	68
29	Tuning the Transparency of Cu₂O with Substitutional Cation Doping. Chemistry of Materials, 2008, 20, 5522-5531.	3.2	67
30	Surface modification of TiO2 with metal oxide nanoclusters: a route to composite photocatalytic materials. Chemical Communications, 2011, 47, 8617.	2.2	66
31	The electronic structure of alkali doped alkaline earth metal oxides: Li doping of MgO studied with DFT-GGA and GGA+U. Surface Science, 2005, 586, 25-37.	0.8	65
32	Loading Effect in Copper(II) Oxide Cluster-Surface-Modified Titanium(IV) Oxide on Visible- and UV-Light Activities. Journal of Physical Chemistry C, 2013, 117, 23848-23857.	1.5	65
33	Surface modification of TiO2 with copper clusters for band gap narrowing. Catalysis Today, 2019, 321-322, 9-17.	2.2	61
34	Low Valence Cation Doping of Bulk Cr₂O₃: Charge Compensation and Oxygen Vacancy Formation. Journal of Physical Chemistry C, 2016, 120, 19160-19174.	1.5	59
35	Effect of chlorine doping on electrical and optical properties of ZnO thin films. Thin Solid Films, 2008, 516, 8146-8149.	0.8	55
36	Density functional theory simulation of titanium migration and reaction with oxygen in the early stages of oxidation of equiatomic NiTi alloy. Biomaterials, 2010, 31, 3439-3448.	5.7	55

#	Article	IF	Citations
37	Defects in Cu2O, CuAlO2 and SrCu2O2 transparent conducting oxides. Thin Solid Films, 2008, 516, 8130-8135.	0.8	54
38	Healing of oxygen vacancies on reduced surfaces of gold-doped ceria. Journal of Chemical Physics, 2009, 130, 144702.	1.2	52
39	Reactivity of metal oxide nanocluster modified rutile and anatase TiO2: Oxygen vacancy formation and CO2 interaction. Applied Catalysis A: General, 2016, 521, 240-249.	2.2	51
40	Electronic coupling in iron oxide-modified TiO2 leads to a reduced band gap and charge separation for visible light active photocatalysis. Physical Chemistry Chemical Physics, 2011, 13, 18194.	1.3	50
41	SnO-nanocluster modified anatase TiO2 photocatalyst: exploiting the Sn(ii) lone pair for a new photocatalyst material with visible light absorption and charge carrier separation. Journal of Materials Chemistry A, 2013, 1, 6670.	5.2	50
42	Reactivity of sub 1 nm supported clusters: (TiO2)n clusters supported on rutile TiO2 (110). Physical Chemistry Chemical Physics, 2011, 13, 4963.	1.3	49
43	Dissociative adsorption of methane on the Cu and Zn doped (111) surface of CeO2. Applied Catalysis B: Environmental, 2016, 197, 324-336.	10.8	49
44	Charge compensation in trivalent cation doped bulk rutile TiO₂. Journal of Physics Condensed Matter, 2011, 23, 334207.	0.7	48
45	Ferroelectricity and Large Piezoelectric Response of AlN/ScN Superlattice. ACS Applied Materials & Interfaces, 2019, 11, 20482-20490.	4.0	47
46	Vibrational properties of CO on ceria surfaces. Surface Science, 2006, 600, 175-178.	0.8	46
47	Charge transfer and formation of reduced Ce3+ upon adsorption of metal atoms at the ceria (110) surface. Journal of Chemical Physics, 2012, 136, 134703.	1.2	45
48	TiO2 nanocluster modified-rutile TiO2 photocatalyst: a first principles investigation. Journal of Materials Chemistry A, 2013, 1, 2515.	5.2	45
49	Unravelling the specific site preference in doping of calcium hydroxyapatite with strontium from ab initio investigations and Rietveld analyses. Physical Chemistry Chemical Physics, 2012, 14, 3435.	1.3	43
50	Photocatalytic Activities of Tin(IV) Oxide Surface-Modified Titanium(IV) Dioxide Show a Strong Sensitivity to the TiO₂ Crystal Form. Journal of Physical Chemistry C, 2012, 116, 12621-12626.	1.5	42
51	Mo doped TiO₂: impact on oxygen vacancies, anatase phase stability and photocatalytic activity. JPhys Materials, 2020, 3, 025008.	1.8	42
52	First-Principles Prediction of New Photocatalyst Materials with Visible-Light Absorption and Improved Charge Separation: Surface Modification of Rutile TiO₂ with Nanoclusters of MgO and Ga₂O₃. ACS Applied Materials & Interfaces, 2012, 4, 5863-5871.	4.0	41
53	Effect of La doping on CO adsorption at ceria surfaces. Journal of Chemical Physics, 2009, 131, 244702.	1.2	40
54	The nature of interfaces and charge trapping sites in photocatalytic mixed-phase TiO2 from first principles modeling. Journal of Chemical Physics, 2015, 142, 024708.	1.2	40

#	Article	IF	Citations
55	Formal quantum efficiencies for the photocatalytic reduction of CO2 in a gas phase batch reactor. Catalysis Today, 2019, 326, 75-81.	2.2	39
56	Impact of electronâ€“electron cusp on configuration interaction energies. Journal of Chemical Physics, 2001, 115, 1626-1634.	1.2	38
57	Doping of ceria surfaces with lanthanum: a DFT +Ustudy. Journal of Physics Condensed Matter, 2010, 22, 135004.	0.7	38
58	Tin oxide-surface modified anatase titanium(<scp>iv</scp>) dioxide with enhanced UV-light photocatalytic activity. Physical Chemistry Chemical Physics, 2012, 14, 705-711.	1.3	36
59	Molecular Metal Oxide Cluster-Surface Modified Titanium(IV) Dioxide Photocatalysts. Australian Journal of Chemistry, 2012, 65, 624.	0.5	36
60	Lead oxide-modified TiO2 photocatalyst: tuning light absorption and charge carrier separation by lead oxidation state. Catalysis Science and Technology, 2013, 3, 2000.	2.1	36
61	Enhancing the oxygen vacancy formation and migration in bulk chromium(<scp>iii</scp>) oxide by alkali metal doping: a change from isotropic to anisotropic oxygen diffusion. Journal of Materials Chemistry A, 2017, 5, 15613-15630.	5.2	36
62	Hybrid density functional theory description of N- and C-doping of NiO. Journal of Chemical Physics, 2011, 134, 224703.	1.2	34
63	Highly Sensitive SERS Detection of Neonicotinoid Pesticides. Complete Raman Spectral Assignment of Clothianidin and Imidacloprid. Journal of Physical Chemistry A, 2020, 124, 7238-7247.	1.1	34
64	Surface and interstitial Ti diffusion at the rutile TiO2(110) surface. Physical Chemistry Chemical Physics, 2010, 12, 9763.	1.3	32
65	Role of surface reconstruction on Cu/TiO2 nanotubes for CO2 conversion. Applied Catalysis B: Environmental, 2019, 255, 117754.	10.8	32
66	A Monte Carlo configuration generation computer program for the calculation of electronic states of atoms, molecules, and quantum dots. Computer Physics Communications, 2000, 131, 142-163.	3.0	31
67	Local Interfacial Structure Influences Charge Localization in Titania Composites: Beyond the Band Alignment Paradigm. Journal of Physical Chemistry C, 2016, 120, 1808-1815.	1.5	31
68	Tuning the electronic structure of the transparent conducting oxide Cu2O. Thin Solid Films, 2008, 516, 1468-1472.	0.8	30
69	Competing Mechanisms in Atomic Layer Deposition of Er₂O₃ versus La₂O₃ from Cyclopentadienyl Precursors. Chemistry of Materials, 2010, 22, 117-129.	3.2	29
70	CO₂ and water activation on ceria nanocluster modified TiO₂ rutile (110). Journal of Materials Chemistry A, 2018, 6, 9139-9152.	5.2	27
71	A first principles investigation of Bi2O3-modified TiO2 for visible light Activated photocatalysis: The role of TiO2 crystal form and the Bi3+ stereochemical lone pair. Materials Science in Semiconductor Processing, 2014, 25, 59-67.	1.9	26
72	Ab Initio Study of the Atomic Level Structure of the Rutile TiO₂(110)â€“Titanium Nitride (TiN) Interface. ACS Applied Materials & Interfaces, 2017, 9, 38089-38100.	4.0	25

#	Article	IF	Citations
73	Alkaline earth metal oxide nanocluster modification of rutile TiO₂ (110) promotes water activation and CO₂ chemisorption. Journal of Materials Chemistry A, 2018, 6, 9451-9466.	5.2	24
74	Direct Evidence of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>Fe</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo mathvariant="bold">+</mml:mo></mml:mrow></mml:msup></mml:math>-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>Fe</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo mathvariant="bold">+</mml:mo></mml:mrow></mml:msup></mml:math>Charge Ordering in the Ferrim...	2.9	23
75	Revisiting the Dependence of the Optical and Mobility Gaps of Hydrogenated Amorphous Silicon on Hydrogen Concentration. Journal of Physical Chemistry C, 2013, 117, 23956-23963.	1.5	23
76	Localization of Photoexcited Electrons and Holes on Low Coordinated Ti and O Sites in Free and Supported TiO₂ Nanoclusters. Journal of Physical Chemistry C, 2014, 118, 27890-27900.	1.5	23
77	Symmetry, delocalization, and molecular conductance. Journal of Chemical Physics, 2005, 122, 044710.	1.2	22
78	Metal oxide nanocluster-modified TiO₂as solar activated photocatalyst materials. Journal of Physics Condensed Matter, 2016, 28, 074006.	0.7	22
79	Multifunctional photo/thermal catalysts for the reduction of carbon dioxide. Catalysis Today, 2017, 280, 65-73.	2.2	22
80	Modification of 1D TiO₂ nanowires with GaO_xN_y by atomic layer deposition for TiO₂@GaO_xN_y coreâ€“shell nanowires with enhanced photoelectrochemical performance. Nanoscale, 2020, 12, 7159-7173.	2.8	22
81	Reassigning the most stable surface of hydroxyapatite to the water resistant hydroxyl terminated (010) surface. Surface Science, 2014, 623, 55-63.	0.8	21
82	Cation doping size effect for methane activation on alkaline earth metal doping of the CeO2 (111) surface. Catalysis Science and Technology, 2016, 6, 3544-3558.	2.1	20
83	Adsorption of CO₂ on Heterostructures of Bi₂O₃ Nanocluster-Modified TiO₂ and the Role of Reduction in Promoting CO₂ Activation. ACS Omega, 2018, 3, 13117-13128.	1.6	20
84	Self-Limiting Temperature Window for Thermal Atomic Layer Etching of HfO₂ and ZrO₂ Based on the Atomic-Scale Mechanism. Chemistry of Materials, 2020, 32, 3414-3426.	3.2	20
85	Formation of Ce3+ at the cerium dioxide (110) surface by doping. Chemical Physics Letters, 2010, 492, 115-118.	1.2	18
86	The atomic level structure of the TiO2â€“NiTi interface. Physical Chemistry Chemical Physics, 2010, 12, 9742.	1.3	18
87	Surface orientation effects in crystallineâ€“amorphous silicon interfaces. Physical Chemistry Chemical Physics, 2012, 14, 15173.	1.3	18
88	Role of the Head and/or Tail Groups of Adsorbed â^'[Xheadâ€group]â€“Alkylâ€“[Xtailâ€group] [X = O(H), S(H), NH(2)] Chains in Controlling the Work Function of the Functionalized H:Si(111) Surface. Journal of Physical Chemistry C, 2015, 119, 11588-11597.	1.5	18
89	Surface Modification of Perfect and Hydroxylated TiO₂ Rutile (110) and Anatase (101) with Chromium Oxide Nanoclusters. ACS Omega, 2017, 2, 6795-6808.	1.6	18
90	Molecular Layer Deposition of â€œMagnesiconeâ€, a Magnesium-based Hybrid Material. Chemistry of Materials, 2020, 32, 4451-4466.	3.2	17

#	Article	IF	Citations
91	Overcoming Pdâ€“TiO₂ Deactivation during H₂ Production from Photoreforming Using Cu@Pd Nanoparticles Supported on TiO₂. ACS Applied Nano Materials, 2021, 4, 3204-3219.	2.4	17
92	Modifying ceria (111) with a TiO2 nanocluster for enhanced reactivity. Journal of Chemical Physics, 2013, 139, 184710.	1.2	16
93	A first principles analysis of the effect of hydrogen concentration in hydrogenated amorphous silicon on the formation of strained Si-Si bonds and the optical and mobility gaps. Journal of Applied Physics, 2014, 115, .	1.1	16
94	Impact of surface hydroxylation in MgO-/SnO-nanocluster modified TiO2 anatase (101) composites on visible light absorption, charge separation and reducibility. Chinese Chemical Letters, 2018, 29, 757-764.	4.8	16
95	Hydrogen evolution on non-metal oxide catalysts. JPhys Energy, 2020, 2, 042002.	2.3	16
96	Cobalt Metal ALD: Understanding the Mechanism and Role of Zinc Alkyl Precursors as Reductants for Low-Resistivity Co Thin Films. Chemistry of Materials, 2021, 33, 5045-5057.	3.2	16
97	Optical and microstructural properties of p-type SrCu2O2: First principles modeling and experimental studies. Thin Solid Films, 2007, 515, 8624-8631.	0.8	15
98	On the interaction of Mg with the (111) and (110) surfaces of ceria. Physical Chemistry Chemical Physics, 2012, 14, 1293-1301.	1.3	15
99	Antimicrobial properties of vertically aligned nano-tubular copper. Materials Letters, 2014, 128, 60-63.	1.3	15
100	Large Piezoelectric Response and Ferroelectricity in Li and V/Nb/Ta Co-Doped w-AlN. ACS Applied Materials & Interfaces, 2021, 13, 944-954.	4.0	15
101	Density Functional Theory with van der Waals Corrections Study of the Adsorption of Alkyl, Alkylthiol, Alkoxyl, and Amino-Alkyl Chains on the H:Si(111) Surface. Langmuir, 2014, 30, 13255-13265.	1.6	14
102	Formation Mechanism of Metalâ€“Moleculeâ€“Metal Junctions: Molecule-Assisted Migration on Metal Defects. Journal of Physical Chemistry C, 2015, 119, 19438-19451.	1.5	14
103	Modifying the band gap and optical properties of Germanium nanowires by surface termination. Applied Surface Science, 2017, 396, 1155-1163.	3.1	14
104	First principles mechanistic study of self-limiting oxidative adsorption of remote oxygen plasma during the atomic layer deposition of alumina. Physical Chemistry Chemical Physics, 2018, 20, 22783-22795.	1.3	14
105	First principles simulations of elastic properties of radiopaque NiTiPt. Journal of Alloys and Compounds, 2015, 630, 54-59.	2.8	13
106	First-principles molecular dynamics simulations of proton diffusion in cubic BaZrO $$_3$$ 3 perovskite under strain conditions. Materials for Renewable and Sustainable Energy, 2016, 5, 1.	1.5	12
107	Enhanced oxidation activity from modified ceria: MnOxâ€“ceria, CrOxâ€“ceria and Mg doped VOxâ€“ceria. Applied Catalysis B: Environmental, 2016, 197, 313-323.	10.8	12
108	Tuning transition metal carbide activity by surface metal alloying: a case study on CO₂capture and activation. Physical Chemistry Chemical Physics, 2018, 20, 22179-22186.	1.3	12

#	Article	IF	Citations
109	Stability of Adsorbed Water on TiO₂â€“TiN Interfaces. A First-Principles and Ab Initio Thermodynamics Investigation. Journal of Physical Chemistry C, 2018, 122, 15395-15408.	1.5	12
110	Activation of Water on MnOx-Nanocluster-Modified Rutile (110) and Anatase (101) TiO2 and the Role of Cation Reduction. Frontiers in Chemistry, 2019, 7, 67.	1.8	12
111	A carbene stabilized precursor for the spatial atomic layer deposition of copper thin films. Chemical Communications, 2020, 56, 13752-13755.	2.2	12
112	First principles investigation of anion-controlled red shift in light absorption in ZnX (X = O, S, Se) nanocluster modified rutile TiO₂. Journal of Materials Chemistry A, 2014, 2, 18796-18805.	5.2	11
113	Predicting Nucleation of Isonicotinamide from the Solventâ€“Solute Interactions of Isonicotinamide in Common Organic Solvents. Journal of Physical Chemistry A, 2018, 122, 3301-3312.	1.1	11
114	Ru passivated and Ru doped Îµ-TaN surfaces as a combined barrier and liner material for copper interconnects: a first principles study. Journal of Materials Chemistry C, 2019, 7, 7959-7973.	2.7	11
115	Modification of TiO₂ with hBN: high temperature anatase phase stabilisation and photocatalytic degradation of 1,4-dioxane. JPhys Materials, 2020, 3, 015009.	1.8	11
116	Rational Development of Guanidinate and Amidinate Based Cerium and Ytterbium Complexes as Atomic Layer Deposition Precursors: Synthesis, Modeling, and Application. Chemistry - A European Journal, 2021, 27, 4913-4926.	1.7	11
117	Charge transfer in Cr adsorption and reaction at the rutile TiO2(110) surface. Physical Chemistry Chemical Physics, 2009, 11, 2156.	1.3	10
118	Coverage and Stability of NH_x-Terminated Cobalt and Ruthenium Surfaces: A First-Principles Investigation. Journal of Physical Chemistry C, 2019, 123, 25166-25175.	1.5	10
119	Direct Visualization of Independent Ta Centers Supported on Two-Dimensional TiO₂ Nanosheets. Nano Letters, 2019, 19, 8103-8108.	4.5	10
120	Surface Modification of Rutile TiO₂ with Alkaline-Earth Oxide Nanoclusters for Enhanced Oxygen Evolution. ACS Applied Nano Materials, 2020, 3, 6017-6033.	2.4	10
121	Predicting the Effect of Dopants on CO₂ Adsorption in Transition Metal Carbides: Case Study on TiC (001). Journal of Physical Chemistry C, 2020, 124, 15969-15976.	1.5	10
122	Inâ€…Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metalâ€“Support Interactions and Câ^'H Bond Activation at Low Temperature. Angewandte Chemie, 2017, 129, 13221-13226.	1.6	9
123	Negative Piezoelectric Coefficient in Ferromagnetic 1H-LaBr₂ Monolayer. ACS Applied Electronic Materials, 2022, 4, 850-855.	2.0	9
124	A basis set study for the calculation of electronic excitations using Monte Carlo configuration interaction. Journal of Chemical Physics, 2001, 114, 15.	1.2	8
125	First principles study of reactions in alucone growth: the role of the organic precursor. Dalton Transactions, 2020, 49, 8710-8721.	1.6	8
126	DFT calculations of the structure and stability of copper clusters on MoS₂. Beilstein Journal of Nanotechnology, 2020, 11, 391-406.	1.5	8

#	Article	IF	Citations
127	A study on the influence of ligand variation on formamidinate complexes of yttrium: new precursors for atomic layer deposition of yttrium oxide. Dalton Transactions, 2021, 50, 12944-12956.	1.6	8
128	Dual promotional effect of Cu_xO clusters grown with atomic layer deposition on TiO₂ for photocatalytic hydrogen production. Catalysis Science and Technology, 2022, 12, 4511-4523.	2.1	8
129	Influence of trivalent doping on point and Frenkel defect formation in bulk chromium (III) oxide. Solid State Ionics, 2017, 307, 51-64.	1.3	7
130	Monolayer Doping of Germanium with Arsenic: A New Chemical Route to Achieve Optimal Dopant Activation. Langmuir, 2020, 36, 9993-10002.	1.6	7
131	On the use of DFT+U to describe the electronic structure of TiO2 nanoparticles: (TiO2)35 as a case study. Journal of Chemical Physics, 2020, 152, 244107.	1.2	7
132	First-principles analysis of the stability of water on oxidised and reduced CuO(111) surfaces. RSC Advances, 2017, 7, 56721-56731.	1.7	6
133	Structure, stability and water adsorption on ultra-thin TiO₂ supported on TiN. Physical Chemistry Chemical Physics, 2019, 21, 25344-25361.	1.3	6
134	The role of Ru passivation and doping on the barrier and seed layer properties of Ru-modified TaN for copper interconnects. Journal of Chemical Physics, 2020, 152, 144701.	1.2	6
135	Band structure engineering of a molecular wire system composed of dimercaptoacetoamidobenzene, its derivatives, and gold clusters. Computational Materials Science, 2003, 27, 166-174.	1.4	5
136	Non-stoichiometric oxide and metal interfaces and reactions. Applied Physics A: Materials Science and Processing, 2009, 96, 543-548.	1.1	5
137	Binary functionalization of H:Si(111) surfaces by alkyl monolayers with different linker atoms enhances monolayer stability and packing. Physical Chemistry Chemical Physics, 2016, 18, 12952-12963.	1.3	5
138	Exploring the Crystal Landscape of 3-Methyl-2-phenylbutyramide: Crystallization of Metastable Racemic Forms from the Stable Conglomerate. Crystal Growth and Design, 2018, 18, 3549-3557.	1.4	5
139	Activation of CO2 at chromia-nanocluster-modified rutile and anatase TiO2. Catalysis Today, 2019, 326, 68-74.	2.2	5
140	Reactions of ruthenium cyclopentadienyl precursor in the metal precursor pulse of Ru atomic layer deposition. Journal of Materials Chemistry C, 2021, 9, 2919-2932.	2.7	5
141	Modification of TiO₂ with metal chalcogenide nanoclusters for hydrogen evolution. JPhys Energy, 2021, 3, 025001.	2.3	5
142	In silico design of a thermal atomic layer etch process of cobalt. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2021, 39, .	0.9	5
143	Atomic/molecular layer deposition of Ti-organic thin films from different aromatic alcohol and amine precursors. Thin Solid Films, 2021, 736, 138896.	0.8	5
144	Role of terminal groups in aromatic molecules on the growth of Al₂O₃-based hybrid materials. Dalton Transactions, 2021, 50, 17583-17593.	1.6	5

#	Article	IF	Citations
145	Control of the Cu morphology on Ru-passivated and Ru-doped TaN surfaces â€“ promoting growth of 2D conducting copper for CMOS interconnects. Chemical Science, 2022, 13, 713-725.	3.7	5
146	Self-limiting nitrogen/hydrogen plasma radical chemistry in plasma-enhanced atomic layer deposition of cobalt. Nanoscale, 2022, 14, 4712-4725.	2.8	5
147	Origin of enhanced thermal atomic layer etching of amorphous HfO₂. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2022, 40, 022604.	0.9	5
148	Mechanism of Thermal Atomic Layer Etch of W Metal Using Sequential Oxidation and Chlorination: A First-Principles Study. ACS Applied Materials & Interfaces, 2020, 12, 36670-36680.	4.0	4
149	Reaction Mechanism of the Metal Precursor Pulse in Plasma-Enhanced Atomic Layer Deposition of Cobalt and the Role of Surface Facets. Journal of Physical Chemistry C, 2020, 124, 11990-12000.	1.5	4
150	Ferromagnetic Europium Sulfide Thin Films: Influence of Precursors on Magneto-Optical Properties. Chemistry of Materials, 2022, 34, 152-164.	3.2	4
151	Photo-dissociation of hydrogen passivated dopants in gallium arsenide. Nuclear Instruments & Methods in Physics Research B, 2002, 186, 234-239.	0.6	3
152	Surface Effects in the Reactivity of Ceria. , 2015, , 159-192.		3
153	Atomic/molecular layer deposition of cerium(<scp>iii</scp>) hybrid thin films using rigid organic precursors. Dalton Transactions, 2022, 51, 5603-5611.	1.6	3
154	Molecular Dynamics Studies of the Phase Transitions of Homopolymers of p-Hydroxybenzoic Acid. Journal of Physical Chemistry B, 1999, 103, 7111-7121.	1.2	2
155	A miniaturised autonomous sensor based on nanowire materials platform: the SiNAPS mote. , 2013, , .		2
156	Non-classical behaviour of higher valence dopants in chromium (III) oxide by a Cr vacancy compensation mechanism. Journal of Physics Condensed Matter, 2017, 29, 415501.	0.7	2
157	Unravelling the Impact of Ta Doping on the Electronic and Structural Properties of Titania: A Combined Theoretical and Experimental Approach. Journal of Physical Chemistry C, 2022, 126, 2285-2297.	1.5	2
158	Atomic Layer Deposition of Intermetallic Fe₄Zn₉ Thin Films from Diethyl Zinc. Chemistry of Materials, 2022, 34, 5241-5248.	3.2	2
159	Component design and testing for a miniaturised autonomous sensor based on a nanowire materials platform. Microsystem Technologies, 2014, 20, 971-988.	1.2	1
160	First Principles Modelling of Surface Modified TiO2 for Water Activation and Oxygen Evolution. ECS Meeting Abstracts, 2020, MA2020-01, 1556-1556.	0.0	1
161	Design of Photocatalysts for CO<inf>2</inf> Reduction from First Principles. , 2018, , .		0
162	Prediction of Co and Ru nanocluster morphology on 2D MoS2 from interaction energies. Beilstein Journal of Nanotechnology, 2021, 12, 704-724.	1.5	0

#	Article	IF	Citations
163	New Materials to Battle the Transistor Interconnect Bottleneck. ECS Meeting Abstracts, 2020, MA2020-01, 1294-1294.	0.0	0
164	DFT Study on Atomic Layer Deposition of Cerium Dioxide on Hydroxylated Titanium Dioxide As Efficient Photocatalyst. ECS Meeting Abstracts, 2020, MA2020-01, 2770-2770.	0.0	0
165	First Principles Simulations of Surface Modified TiO2 for CO2 Activation. ECS Meeting Abstracts, 2020, MA2020-01, 2762-2762.	0.0	0
166	Structure and Stability of Cu_n Clusters (n = 1-4) Adsorbed on Stoichiometric and Defective 2D MoS₂. ECS Meeting Abstracts, 2020, MA2020-01, 2924-2924.	0.0	0
167	Modelling the Atomic Layer Deposition of Cobalt and Ruthenium on NHx-Terminated Metal Surfaces. ECS Meeting Abstracts, 2020, MA2020-01, 1295-1295.	0.0	0
168	Surface Modification of Rutile TiO2 with Metal Chalcogenides for Hydrogen Evolution. ECS Meeting Abstracts, 2020, MA2020-01, 1527-1527.	0.0	0