Michael Nolan

List of Publications by Year in Descending Order

160 papers	6,180 citations	40 h-index	75 g-index
244 ext. papers	6,927 ext. citations	5.4 avg, IF	6.44 L-index

#	Paper	IF	Citations
160	Negative Piezoelectric Coefficient in Ferromagnetic 1H-LaBr Monolayer.. *ACS Applied Electronic Materials*, **2022**, 4, 850-855	4	0
159	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	3.8	1
158	Control of the Cu morphology on Ru-passivated and Ru-doped TaN surfaces - promoting growth of 2D conducting copper for CMOS interconnects.. *Chemical Science*, **2022**, 13, 713-725	9.4	1
157	Origin of enhanced thermal atomic layer etching of amorphous HfO2. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2022**, 40, 022604	2.9	1
156	Ferromagnetic Europium Sulfide Thin Films: Influence of Precursors on Magneto-Optical Properties. *Chemistry of Materials*, **2022**, 34, 152-164	9.6	0
155	Role of terminal groups in aromatic molecules on the growth of AlO-based hybrid materials. *Dalton Transactions*, **2021**, 50, 17583-17593	4.3	1
154	Large Piezoelectric Response and Ferroelectricity in Li and V/Nb/Ta Co-Doped w-AlN. *ACS Applied Materials & Interfaces*, **2021**, 13, 944-954	9.5	4
153	Modification of TiO2 with metal chalcogenide nanoclusters for hydrogen evolution. *JPhys Energy*, **2021**, 3, 025001	4.9	2
152	Overcoming Pd□TiO2 Deactivation during H2 Production from Photoreforming Using Cu@Pd Nanoparticles Supported on TiO2. *ACS Applied Nano Materials*, **2021**, 4, 3204-3219	5.6	9
151	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, 022603	2.9	2
150	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	9.6	3
149	Insights into Photocatalysis from Computational Chemistry **2021**, 127-154		
148	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	4.8	3
147	Reactions of ruthenium cyclopentadienyl precursor in the metal precursor pulse of Ru atomic layer deposition. *Journal of Materials Chemistry C*, **2021**, 9, 2919-2932	7.1	0
146	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	4.3	1
145	Prediction of Co and Ru nanocluster morphology on 2D MoS from interaction energies. *Beilstein Journal of Nanotechnology*, **2021**, 12, 704-724	3	
144	Atomic/molecular layer deposition of Ti-organic thin films from different aromatic alcohol and amine precursors. *Thin Solid Films*, **2021**, 736, 138896	2.2	3

143	Molecular Layer Deposition of Magnesicone, a Magnesium-based Hybrid Material. *Chemistry of Materials*, **2020**, 32, 4451-4466	9.6	8
142	Surface Modification of Rutile TiO2 with Alkaline-Earth Oxide Nanoclusters for Enhanced Oxygen Evolution. *ACS Applied Nano Materials*, **2020**, 3, 6017-6033	5.6	8
141	First principles study of reactions in alucone growth: the role of the organic precursor. *Dalton Transactions*, **2020**, 49, 8710-8721	4.3	3
140	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	3.8	5
139	On the use of DFT+U to describe the electronic structure of TiO nanoparticles: (TiO) as a case study. *Journal of Chemical Physics*, **2020**, 152, 244107	3.9	2
138	Mo doped TiO2: impact on oxygen vacancies, anatase phase stability and photocatalytic activity. *JPhys Materials*, **2020**, 3, 025008	4.2	18
137	Modification of 1D TiO nanowires with GaON by atomic layer deposition for TiO@GaON core-shell nanowires with enhanced photoelectrochemical performance. *Nanoscale*, **2020**, 12, 7159-7173	7.7	11
136	DFT calculations of the structure and stability of copper clusters on MoS. *Beilstein Journal of Nanotechnology*, **2020**, 11, 391-406	3	6
135	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	3.9	4
134	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	9.6	14
133	Structure and Stability of Cun Clusters (n = 1-4) Adsorbed on Stoichiometric and Defective 2D MoS2. *ECS Meeting Abstracts*, **2020**, MA2020-01, 2924-2924	0	
132	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	3.8	2
131	Modification of TiO2 with hBN: high temperature anatase phase stabilisation and photocatalytic degradation of 1,4-dioxane. *JPhys Materials*, **2020**, 3, 015009	4.2	5
130	A carbene stabilized precursor for the spatial atomic layer deposition of copper thin films. *Chemical Communications*, **2020**, 56, 13752-13755	5.8	3
129	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	9.5	2
128	Hydrogen evolution on non-metal oxide catalysts. *JPhys Energy*, **2020**, 2, 042002	4.9	9
127	Highly Sensitive SERS Detection of Neonicotinoid Pesticides. Complete Raman Spectral Assignment of Clothianidin and Imidacloprid. *Journal of Physical Chemistry A*, **2020**, 124, 7238-7247	2.8	13
126	Monolayer Doping of Germanium with Arsenic: A New Chemical Route to Achieve Optimal Dopant Activation. *Langmuir*, **2020**, 36, 9993-10002	4	2

125	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	21.8	59
124	Ru passivated and Ru doped 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	7.1	7
123	Ferroelectricity and Large Piezoelectric Response of AlN/ScN Superlattice. *ACS Applied Materials & Interfaces*, **2019**, 11, 20482-20490	9.5	22
122	Role of surface reconstruction on Cu/TiO2 nanotubes for CO2 conversion. *Applied Catalysis B: Environmental*, **2019**, 255, 117754	21.8	14
121	Indium-Doped TiO2 Photocatalysts with High-Temperature Anatase Stability. *Journal of Physical Chemistry C*, **2019**, 123, 21083-21096	3.8	39
120	Coverage and Stability of NHx-Terminated Cobalt and Ruthenium Surfaces: A First-Principles Investigation. *Journal of Physical Chemistry C*, **2019**, 123, 25166-25175	3.8	5
119	Direct Visualization of Independent Ta Centers Supported on Two-Dimensional TiO Nanosheets. *Nano Letters*, **2019**, 19, 8103-8108	11.5	7
118	Activation of Water on MnO-Nanocluster-Modified Rutile (110) and Anatase (101) TiO and the Role of Cation Reduction. *Frontiers in Chemistry*, **2019**, 7, 67	5	6
117	Structure, stability and water adsorption on ultra-thin TiO supported on TiN. *Physical Chemistry Chemical Physics*, **2019**, 21, 25344-25361	3.6	2
116	Activation of CO2 at chromia-nanocluster-modified rutile and anatase TiO2. *Catalysis Today*, **2019**, 326, 68-74	5.3	2
115	Formal quantum efficiencies for the photocatalytic reduction of CO2 in a gas phase batch reactor. *Catalysis Today*, **2019**, 326, 75-81	5.3	27
114	Surface modification of TiO2 with copper clusters for band gap narrowing. *Catalysis Today*, **2019**, 321-322, 9-17	5.3	47
113	Predicting Nucleation of Isonicotinamide from the Solvent-Solute Interactions of Isonicotinamide in Common Organic Solvents. *Journal of Physical Chemistry A*, **2018**, 122, 3301-3312	2.8	9
112	Advances in the Development of Novel Photocatalysts for Detoxification **2018**, 283-327		1
111	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	3.5	2
110	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	13	16
109	CO2 and water activation on ceria nanocluster modified TiO2 rutile (110). *Journal of Materials Chemistry A*, **2018**, 6, 9139-9152	13	19
108	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	3.6	8

107	Tuning transition metal carbide activity by surface metal alloying: a case study on CO capture and activation. *Physical Chemistry Chemical Physics*, **2018**, 20, 22179-22186	3.6	8
106	Stability of Adsorbed Water on TiO2−TiN Interfaces. A First-Principles and Ab Initio Thermodynamics Investigation. *Journal of Physical Chemistry C*, **2018**, 122, 15395-15408	3.8	11
105	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	8.1	12
104	Cu-Doped TiO2: Visible Light Assisted Photocatalytic Antimicrobial Activity. *Applied Sciences (Switzerland)*, **2018**, 8, 2067	2.6	94
103	Adsorption of CO on Heterostructures of BiO Nanocluster-Modified TiO and the Role of Reduction in Promoting CO Activation. *ACS Omega*, **2018**, 3, 13117-13128	3.9	12
102	Influence of trivalent doping on point and Frenkel defect formation in bulk chromium (III) oxide. *Solid State Ionics*, **2017**, 307, 51-64	3.3	4
101	Spinel-Structured ZnCr2O4 with Excess Zn Is the Active ZnO/Cr2O3 Catalyst for High-Temperature Methanol Synthesis. *ACS Catalysis*, **2017**, 7, 7610-7622	13.1	61
100	Surface Modification of Perfect and Hydroxylated TiO Rutile (110) and Anatase (101) with Chromium Oxide Nanoclusters. *ACS Omega*, **2017**, 2, 6795-6808	3.9	16
99	Ab Initio Study of the Atomic Level Structure of the Rutile TiO(110)-Titanium Nitride (TiN) Interface. *ACS Applied Materials & Interfaces*, **2017**, 9, 38089-38100	9.5	17
98	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	1.8	2
97	In Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metal−Support Interactions and C−H Bond Activation at Low Temperature. *Angewandte Chemie*, **2017**, 129, 13221-13226	3.6	7
96	In Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metal-Support Interactions and C-H Bond Activation at Low Temperature. *Angewandte Chemie - International Edition*, **2017**, 56, 13041-13046	16.4	90
95	Enhancing the oxygen vacancy formation and migration in bulk chromium(III) oxide by alkali metal doping: a change from isotropic to anisotropic oxygen diffusion. *Journal of Materials Chemistry A*, **2017**, 5, 15613-15630	13	22
94	Modifying the band gap and optical properties of Germanium nanowires by surface termination. *Applied Surface Science*, **2017**, 396, 1155-1163	6.7	10
93	Multifunctional photo/thermal catalysts for the reduction of carbon dioxide. *Catalysis Today*, **2017**, 280, 65-73	5.3	18
92	First-principles analysis of the stability of water on oxidised and reduced CuO(111) surfaces. *RSC Advances*, **2017**, 7, 56721-56731	3.7	5
91	Low Valence Cation Doping of Bulk Cr2O3: Charge Compensation and Oxygen Vacancy Formation. *Journal of Physical Chemistry C*, **2016**, 120, 19160-19174	3.8	36
90	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, 12952-63	3.6	5

89	Enhanced oxidation activity from modified ceria: MnOx□eria, CrOx□eria and Mg doped VOx□eria. *Applied Catalysis B: Environmental*, **2016**, 197, 313-323	21.8	8
88	Local Interfacial Structure Influences Charge Localization in Titania Composites: Beyond the Band Alignment Paradigm. *Journal of Physical Chemistry C*, **2016**, 120, 1808-1815	3.8	26
87	Reactivity of metal oxide nanocluster modified rutile and anatase TiO2: Oxygen vacancy formation and CO2 interaction. *Applied Catalysis A: General*, **2016**, 521, 240-249	5.1	39
86	Metal oxide nanocluster-modified TiO2 as solar activated photocatalyst materials. *Journal of Physics Condensed Matter*, **2016**, 28, 074006	1.8	17
85	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	5.5	14
84	Design of Novel Visible Light Active Photocatalyst Materials: Surface Modified TiO2. *Advanced Materials*, **2016**, 28, 5425-46	24	119
83	Dissociative adsorption of methane on the Cu and Zn doped (111) surface of CeO2. *Applied Catalysis B: Environmental*, **2016**, 197, 324-336	21.8	38
82	First-principles molecular dynamics simulations of proton diffusion in cubic BaZrO(_3) perovskite under strain conditions. *Materials for Renewable and Sustainable Energy*, **2016**, 5, 1	4.7	7
81	Formation Mechanism of Metal□Molecule□Metal Junctions: Molecule-Assisted Migration on Metal Defects. *Journal of Physical Chemistry C*, **2015**, 119, 19438-19451	3.8	10
80	Role of the Head and/or Tail Groups of Adsorbed [X□head group]□Alkyl□[X□tail 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	3.8	17
79	Surface Effects in the Reactivity of Ceria **2015**, 159-192		3
78	First principles simulations of elastic properties of radiopaque NiTiPt. *Journal of Alloys and Compounds*, **2015**, 630, 54-59	5.7	11
77	The nature of interfaces and charge trapping sites in photocatalytic mixed-phase TiO2 from first principles modeling. *Journal of Chemical Physics*, **2015**, 142, 024708	3.9	35
76	Component design and testing for a miniaturised autonomous sensor based on a nanowire materials platform. *Microsystem Technologies*, **2014**, 20, 971-988	1.7	
75	Molecular-Scale Transition Metal Oxide Nanocluster Surface-Modified Titanium Dioxide as Solar-Activated Environmental Catalysts. *Journal of Physical Chemistry C*, **2014**, 118, 12077-12086	3.8	69
74	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	4.3	21
73	Reduction mechanisms of the CuO(111) surface through surface oxygen vacancy formation and hydrogen adsorption. *Physical Chemistry Chemical Physics*, **2014**, 16, 3036-46	3.6	116
72	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, 13255-65	4	13

71	Key scientific challenges in current rechargeable non-aqueous Li-O2 batteries: experiment and theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 12093-130	3.6	115
70	Reassigning the most stable surface of hydroxyapatite to the water resistant hydroxyl terminated (010) surface. *Surface Science*, **2014**, 623, 55-63	1.8	17
69	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	13	10
68	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, 203711	2.5	11
67	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	3.8	20
66	Antimicrobial properties of vertically aligned nano-tubular copper. *Materials Letters*, **2014**, 128, 60-63	3.3	14
65	Direct evidence of Fe(2+)-Fe3+ charge ordering in the ferrimagnetic hematite-ilmenite Fe(1.35)Ti(0.65)O(3-δ) thin films. *Physical Review Letters*, **2013**, 111, 167202	7.4	21
64	Lead oxide-modified TiO2 photocatalyst: tuning light absorption and charge carrier separation by lead oxidation state. *Catalysis Science and Technology*, **2013**, 3, 2000	5.5	28
63	Modifying ceria (111) with a TiO2 nanocluster for enhanced reactivity. *Journal of Chemical Physics*, **2013**, 139, 184710	3.9	12
62	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	13	40
61	TiO2 nanocluster modified-rutile TiO2 photocatalyst: a first principles investigation. *Journal of Materials Chemistry A*, **2013**, 1, 2515	13	35
60	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	3.8	61
59	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	3.8	17
58	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	3.8	61
57	A miniaturised autonomous sensor based on nanowire materials platform: the SiNAPS mote **2013**,		1
56	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, 3435-43	3.6	35
55	Tin oxide-surface modified anatase titanium(IV) dioxide with enhanced UV-light photocatalytic activity. *Physical Chemistry Chemical Physics*, **2012**, 14, 705-11	3.6	32
54	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	3.8	38

53	Surface orientation effects in crystalline-amorphous silicon interfaces. *Physical Chemistry Chemical Physics*, **2012**, 14, 15173-9	3.6	11
52	Molecular Metal Oxide Cluster-Surface Modified Titanium(IV) Dioxide Photocatalysts. *Australian Journal of Chemistry*, **2012**, 65, 624	1.2	28
51	First-principles prediction of new photocatalyst materials with visible-light absorption and improved charge separation: surface modification of rutile TiO with nanoclusters of MgO and Ga *ACS Applied Materials & Interfaces*, **2012**, 4, 5863-71	9.5	38
50	Charge transfer and formation of reduced Ce3+ upon adsorption of metal atoms at the ceria (110) surface. *Journal of Chemical Physics*, **2012**, 136, 134703	3.9	37
49	On the interaction of Mg with the (111) and (110) surfaces of ceria. *Physical Chemistry Chemical Physics*, **2012**, 14, 1293-301	3.6	14
48	Surface modification of TiO2 with metal oxide nanoclusters: a route to composite photocatalytic materials. *Chemical Communications*, **2011**, 47, 8617-9	5.8	60
47	Enhanced oxygen vacancy formation in ceria (111) and (110) surfaces doped with divalent cations. *Journal of Materials Chemistry*, **2011**, 21, 9160		121
46	Hybrid density functional theory description of N- and C-doping of NiO. *Journal of Chemical Physics*, **2011**, 134, 224703	3.9	27
45	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	3.8	74
44	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, 18194-9	3.6	48
43	Reactivity of sub 1 nm supported clusters: (TiO2)n clusters supported on rutile TiO2 (110). *Physical Chemistry Chemical Physics*, **2011**, 13, 4963-73	3.6	43
42	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	3.8	84
41	Charge compensation in trivalent cation doped bulk rutile TiO2. *Journal of Physics Condensed Matter*, **2011**, 23, 334207	1.8	37
40	Competing Mechanisms in Atomic Layer Deposition of Er2O3 versus La2O3 from Cyclopentadienyl Precursors. *Chemistry of Materials*, **2010**, 22, 117-129	9.6	26
39	Doping of ceria surfaces with lanthanum: a DFT + U study. *Journal of Physics Condensed Matter*, **2010**, 22, 135004	1.8	36
38	The atomic level structure of the TiO(2)-NiTi interface. *Physical Chemistry Chemical Physics*, **2010**, 12, 9742-50	3.6	18
37	Surface and interstitial Ti diffusion at the rutile TiO(2)(110) surface. *Physical Chemistry Chemical Physics*, **2010**, 12, 9763-71	3.6	27
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, 3439-48	15.6	45

35	Formation of Ce3+ at the cerium dioxide (110) surface by doping. *Chemical Physics Letters*, **2010**, 492, 115-118	2.5	16
34	Hybrid density functional theory description of oxygen vacancies in the CeO2 (110) and (100) surfaces. *Chemical Physics Letters*, **2010**, 499, 126-130	2.5	63
33	Effect of La doping on CO adsorption at ceria surfaces. *Journal of Chemical Physics*, **2009**, 131, 244702	3.9	38
32	Healing of oxygen vacancies on reduced surfaces of gold-doped ceria. *Journal of Chemical Physics*, **2009**, 130, 144702	3.9	50
31	Non-stoichiometric oxide and metal interfaces and reactions. *Applied Physics A: Materials Science and Processing*, **2009**, 96, 543-548	2.6	4
30	Molecular Adsorption on the Doped (110) Ceria Surface. *Journal of Physical Chemistry C*, **2009**, 113, 2425-2432	3.8	86
29	Charge transfer in Cr adsorption and reaction at the rutile TiO2(110) surface. *Physical Chemistry Chemical Physics*, **2009**, 11, 2156-60	3.6	9
28	Tuning the Transparency of Cu2O with Substitutional Cation Doping. *Chemistry of Materials*, **2008**, 20, 5522-5531	9.6	56
27	Electronic structure of point defects in controlled self-doping of the TiO2 (110) surface: Combined photoemission spectroscopy and density functional theory study. *Physical Review B*, **2008**, 77,	3.3	122
26	Effect of chlorine doping on electrical and optical properties of ZnO thin films. *Thin Solid Films*, **2008**, 516, 8146-8149	2.2	48
25	Vacancy formation and CO adsorption on gold-doped ceria surfaces. *Surface Science*, **2008**, 602, 2734-2742	2.1	115
24	Tuning the electronic structure of the transparent conducting oxide Cu2O. *Thin Solid Films*, **2008**, 516, 1468-1472	2.2	29
23	Defects in Cu2O, CuAlO2 and SrCu2O2 transparent conducting oxides. *Thin Solid Films*, **2008**, 516, 8130-8135	2.2	49
22	Silicon nanowire band gap modification. *Nano Letters*, **2007**, 7, 34-8	11.5	192
21	Surface Sensitivity in Lithium-Doping of MgO: A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. *Journal of Physical Chemistry C*, **2007**, 111, 7971-7979	3.8	91
20	Optical and microstructural properties of p-type SrCu2O2: First principles modeling and experimental studies. *Thin Solid Films*, **2007**, 515, 8624-8631	2.2	15
19	Vibrational properties of CO on ceria surfaces. *Surface Science*, **2006**, 600, 175-178	1.8	42
18	The surface dependence of CO adsorption on Ceria. *Journal of Physical Chemistry B*, **2006**, 110, 16600-6	3.4	157

17	Reduction of NO2 on ceria surfaces. *Journal of Physical Chemistry B*, **2006**, 110, 2256-62	3.4	115
16	CeO2 catalysed conversion of CO, NO2 and NO from first principles energetics. *Physical Chemistry Chemical Physics*, **2006**, 8, 216-8	3.6	98
15	The p-type conduction mechanism in Cu2O: a first principles study. *Physical Chemistry Chemical Physics*, **2006**, 8, 5350-8	3.6	247
14	Hole localization in Al doped silica: A DFT + U description. *Journal of Chemical Physics*, **2006**, 125, 144701	3.9	101
13	Oxygen vacancy formation and migration in ceria. *Solid State Ionics*, **2006**, 177, 3069-3074	3.3	256
12	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	1.8	576
11	The electronic structure of oxygen vacancy defects at the low index surfaces of ceria. *Surface Science*, **2005**, 595, 223-232	1.8	585
10	Symmetry, delocalization, and molecular conductance. *Journal of Chemical Physics*, **2005**, 122, 44710	3.9	21
9	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	1.8	57
8	Band structure engineering of a molecular wire system composed of dimercaptoacetoamidobenzene, its derivatives, and gold clusters. *Computational Materials Science*, **2003**, 27, 166-174	3.2	5
7	Photo-dissociation of hydrogen passivated dopants in gallium arsenide. *Nuclear Instruments & Methods in Physics Research B*, **2002**, 186, 234-239	1.2	3
6	Interactions between Thiol Molecular Linkers and the Au13 Nanoparticle. *Journal of Physical Chemistry B*, **2002**, 106, 5931-5937	3.4	78
5	A basis set study for the calculation of electronic excitations using Monte Carlo configuration interaction. *Journal of Chemical Physics*, **2001**, 114, 15	3.9	8
4	Impact of electron□electron cusp on configuration interaction energies. *Journal of Chemical Physics*, **2001**, 115, 1626-1634	3.9	37
3	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	4.2	25
2	Molecular Dynamics Studies of the Phase Transitions of Homopolymers of p-Hydroxybenzoic Acid. *Journal of Physical Chemistry B*, **1999**, 103, 7111-7121	3.4	2
1	Cu Doped TiO2: Visible Light Assisted Photocatalytic Antimicrobial Activity and High Temperature Anatase Stability		3