Simon D Elliott

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

88	2,957	29	52
papers	citations	h-index	g-index
94	3,278	4.9	5.62
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
88	Spontaneous etching of B2O3 by HF gas studied using infrared spectroscopy, mass spectrometry, and density functional theory. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2022**, 40, 022601	2.9	2
87	Prediction and Validation of the Process Window for Atomic Layer Etching: HF Exposure on TiO2. *Journal of Physical Chemistry C*, **2021**, 125, 25589-25599	3.8	4
86	Combining Experimental and DFT Investigation of the Mechanism Involved in Thermal Etching of Titanium Nitride Using Alternate Exposures of NbF5 and CCl4, or CCl4 Only. *Advanced Materials Interfaces*, **2021**, 8, 2101085	4.6	2
85	Thermal Atomic Layer Etching of Aluminum Oxide (Al2O3) Using Sequential Exposures of Niobium Pentafluoride (NbF5) and Carbon Tetrachloride (CCl4): A Combined Experimental and Density Functional Theory Study of the Etch Mechanism. *Chemistry of Materials*, **2021**, 33, 2883-2893	9.6	6
84	Quantifying the Extent of Ligand Incorporation and the Effect on Properties of TiO2 Thin Films Grown by Atomic Layer Deposition Using an Alkoxide or an Alkylamide. *Chemistry of Materials*, **2020** , 32, 1393-1407	9.6	14
83	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
82	A Secondary Reaction Pathway for the Alumina Atomic Layer Deposition Process with Trimethylaluminum and Water, Revealed by Full-Range, Time-Resolved In Situ Mass Spectrometry. *Journal of Physical Chemistry C*, **2020**, 124, 26443-26454	3.8	3
81	Atomic Layer Deposition of Localized Boron- and Hydrogen-Doped Aluminum Oxide Using Trimethyl Borate as a Dopant Precursor. *Chemistry of Materials*, **2020**, 32, 4152-4165	9.6	1
80	Atomic layer deposition of silicon-based dielectrics for semiconductor manufacturing: Current status and future outlook. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2019**, 37, 060904	2.9	43
79	Understanding the Mechanism of SiC Plasma-Enhanced Chemical Vapor Deposition (PECVD) and Developing Routes toward SiC Atomic Layer Deposition (ALD) with Density Functional Theory. *ACS Applied Materials & Interfaces*, **2018**, 10, 15216-15225	9.5	13
78	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
77	Modeling the Chemical Mechanism of the Thermal Atomic Layer Etch of Aluminum Oxide: A Density Functional Theory Study of Reactions during HF Exposure. *Chemistry of Materials*, **2018**, 30, 5912-5922	9.6	32
76	Kinetic Monte Carlo Study of the Atomic Layer Deposition of Zinc Oxide. *Journal of Physical Chemistry C*, **2018**, 122, 27044-27058	3.8	11
75	Classification of processes for the atomic layer deposition of metals based on mechanistic information from density functional theory calculations. *Journal of Chemical Physics*, **2017**, 146, 052822	3.9	22
74	Reversible and Irreversible Reactions of Trimethylaluminum with Common Organic Functional Groups as a Model for Molecular Layer Deposition and Vapor Phase Infiltration. *Advanced Materials Interfaces*, **2017**, 4, 1700237	4.6	24
73	Investigating routes toward atomic layer deposition of silicon carbide: Ab initio screening of potential silicon and carbon precursors. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2017**, 35, 01B103	2.9	8
72	Suppressing the Thermal and Ultraviolet Sensitivity of Kevlar by Infiltration and Hybridization with ZnO. *Chemistry of Materials*, **2017**, 29, 10068-10074	9.6	32

71	Kinetics and Coverage Dependent Reaction Mechanisms of the Copper Atomic Layer Deposition from Copper Dimethylamino-2-propoxide and Diethylzinc. *Chemistry of Materials*, **2016**, 28, 6282-6295	9.6	12
70	The role of local chemical hardness and van der Waals interactions in the anionic polymerization of alkyl cyanoacrylates. *Polymer Chemistry*, **2016**, 7, 3236-3243	4.9	5
69	Modeling Mechanism and Growth Reactions for New Nanofabrication Processes by Atomic Layer Deposition. *Advanced Materials*, **2016**, 28, 5367-80	24	48
68	Precursor Adsorption on Copper Surfaces as the First Step during the Deposition of Copper: A Density Functional Study with van der Waals Correction. *Journal of Physical Chemistry C*, **2015**, 119, 9375-9385	3.8	10
67	Quantum chemical and solution phase evaluation of metallocenes as reducing agents for the prospective atomic layer deposition of copper. *Dalton Transactions*, **2015**, 44, 10188-99	4.3	6
66	Quantum Chemical Study of the Effect of Precursor Stereochemistry on Dissociative Chemisorption and Surface Redox Reactions During the Atomic Layer Deposition of the Transition Metal Copper. *Journal of Physical Chemistry C*, **2015**, 119, 5914-5927	3.8	12
65	Role of Surface Termination in Atomic Layer Deposition of Silicon Nitride. *Journal of Physical Chemistry Letters*, **2015**, 6, 3610-4	6.4	40
64	Reductive elimination of hypersilyl halides from zinc(II) complexes. Implications for electropositive metal thin film growth. *Inorganic Chemistry*, **2015**, 54, 7-9	5.1	6
63	Cooperation between adsorbates accounts for the activation of atomic layer deposition reactions. *Nanoscale*, **2015**, 7, 6311-8	7.7	43
62	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
61	Effect of reaction mechanism on precursor exposure time in atomic layer deposition of silicon oxide and silicon nitride. *ACS Applied Materials & Interfaces*, **2014**, 6, 10534-41	9.5	60
60	Decomposition of Metal Alkylamides, Alkyls, and Halides at Reducible Oxide Surfaces: Mechanism of ▯Clean-up▯During Atomic Layer Deposition of Dielectrics onto III▯V Substrates. *Chemistry of Materials*, **2014**, 26, 2427-2437	9.6	15
59	Copper reduction and atomic layer deposition by oxidative decomposition of formate by hydrazine. *RSC Advances*, **2014**, 4, 34448-34453	3.7	15
58	Studying chemical vapor deposition processes with theoretical chemistry. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	36
57	Atomistic kinetic Monte Carlo study of atomic layer deposition derived from density functional theory. *Journal of Computational Chemistry*, **2014**, 35, 244-59	3.5	52
56	First-principles study of oxygen and aluminum defects in ▯Si3N4: Compensation and charge trapping. *Computational Materials Science*, **2014**, 81, 178-183	3.2	11
55	First-Principles Investigation of C▯H Bond Scission and Formation Reactions in Ethane, Ethene, and Ethyne Adsorbed on Ru(0001). *Journal of Physical Chemistry C*, **2014**, 118, 26683-26694	3.8	21
54	Copper(I) carbene hydride complexes acting both as reducing agent and precursor for Cu ALD: a study through density functional theory. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	9

53	ALD Simulations **2014**, 47-69		2
52	Multiple Proton Diffusion and Film Densification in Atomic Layer Deposition Modeled by Density Functional Theory. *Chemistry of Materials*, **2013**, 25, 878-889	9.6	32
51	Deposition of Copper by Plasma-Enhanced Atomic Layer Deposition Using a Novel N-Heterocyclic Carbene Precursor. *Chemistry of Materials*, **2013**, 25, 1132-1138	9.6	39
50	Density functional theory predictions of the composition of atomic layer deposition-grown ternary oxides. *ACS Applied Materials & Interfaces*, **2013**, 5, 3704-15	9.5	29
49	Modeling of Precursors for Atomic Layer Deposition of Magnesium and Calcium Oxide. *Chemical Vapor Deposition*, **2013**, 19, 117-124		10
48	TEMAZ/O3 atomic layer deposition process with doubled growth rate and optimized interface properties in metal‐insulator‐metal capacitors. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2013**, 31, 01A123	2.9	17
47	First principles simulation of reaction steps in the atomic layer deposition of titania: dependence of growth on Lewis acidity of titanocene precursor. *Physical Chemistry Chemical Physics*, **2012**, 14, 7954-64	3.6	20
46	Mechanisms for Substrate-Enhanced Growth during the Early Stages of Atomic Layer Deposition of Alumina onto Silicon Nitride Surfaces. *Chemistry of Materials*, **2012**, 24, 1080-1090	9.6	15
45	Mechanism for the atomic layer deposition of copper using diethylzinc as the reducing agent: a density functional theory study using gas-phase molecules as a model. *Journal of Physical Chemistry A*, **2012**, 116, 8893-901	2.8	29
44	First-Principles Modeling of the “Clean-Up” of Native Oxides during Atomic Layer Deposition onto III‐V Substrates. *Journal of Physical Chemistry C*, **2012**, 116, 643-654	3.8	45
43	Atomic-scale simulation of ALD chemistry. *Semiconductor Science and Technology*, **2012**, 27, 074008	1.8	72
42	Native defects in hexagonal β-Si3N4 studied using density functional theory calculations. *Physical Review B*, **2011**, 83,	3.3	30
41	Understanding ’clean-up’ of III-V native oxides during atomic layer deposition using bulk first principles models. *Journal of Nanoscience and Nanotechnology*, **2011**, 11, 8246-50	1.3	5
40	TiCp*(OMe)3 versus Ti(OMe)4 in atomic layer deposition of TiO2 with water--ab initio modelling of atomic layer deposition surface reactions. *Journal of Nanoscience and Nanotechnology*, **2011**, 11, 8089-93	1.3	14
39	Structural and energetic origin of defects at the interface between germanium and a high-k dielectric from first principles. *Applied Physics Letters*, **2011**, 98, 082904	3.4	3
38	(Invited) Reaction Mechanisms in ALD of Ternary Oxides. *ECS Transactions*, **2011**, 41, 175-183	1	14
37	Competing Mechanisms in Atomic Layer Deposition of Er2O3 versus La2O3 from Cyclopentadienyl Precursors. *Chemistry of Materials*, **2010**, 22, 117-129	9.6	26
36	Thermal stability of precursors for atomic layer deposition of TiO2, ZrO2, and HfO2: an ab initio study of alpha-hydrogen abstraction in bis-cyclopentadienyl dimethyl complexes. *Journal of Physical Chemistry A*, **2010**, 114, 1879-86	2.8	16

35	Mechanism, products, and growth rate of atomic layer deposition of noble metals. *Langmuir*, **2010**, 26, 9179-82	4	50
34	Non-stoichiometric oxide and metal interfaces and reactions. *Applied Physics A: Materials Science and Processing*, **2009**, 96, 543-548	2.6	4
33	Orientation of individual C_{60} molecules adsorbed on Cu(111): Low-temperature scanning tunneling microscopy and density functional calculations. *Physical Review B*, **2008**, 77,	3.3	66
32	Chiral shells and achiral cores in CdS quantum dots. *Nano Letters*, **2008**, 8, 2452-7	11.5	159
31	Tuning the Transparency of Cu_2O with Substitutional Cation Doping. *Chemistry of Materials*, **2008**, 20, 5522-5531	9.6	56
30	Deposition of ZrO_2 and HfO_2 thin films by liquid injection MOCVD and ALD using ansa-metallocene zirconium and hafnium precursors. *Journal of Materials Chemistry*, **2008**, 18, 4561		37
29	Electronic structure of point defects in controlled self-doping of the TiO_2 (110) surface: Combined photoemission spectroscopy and density functional theory study. *Physical Review B*, **2008**, 77,	3.3	122
28	Tuning the electronic structure of the transparent conducting oxide Cu_2O. *Thin Solid Films*, **2008**, 516, 1468-1472	2.2	29
27	Improving ALD growth rate via ligand basicity: Quantum chemical calculations on lanthanum precursors. *Surface and Coatings Technology*, **2007**, 201, 9076-9081	4.4	27
26	Optical and microstructural properties of p-type $SrCu_2O_2$: First principles modeling and experimental studies. *Thin Solid Films*, **2007**, 515, 8624-8631	2.2	15
25	An Ab Initio Evaluation of Cyclopentadienyl Precursors for the Atomic Layer Deposition of Hafnia and Zirconia. *ECS Transactions*, **2007**, 11, 113-121	1	2
24	Atomic scale model interfaces between high-k hafnium silicates and silicon. *Physical Review B*, **2007**, 75,	3.3	23
23	Stress in silicon interlayers at the SiO_x[illegible]Ge interface. *Applied Physics Letters*, **2007**, 90, 143511	3.4	2
22	Mechanism for zirconium oxide atomic layer deposition using bis(methylcyclopentadienyl)methoxymethyl zirconium. *Applied Physics Letters*, **2007**, 91, 253123	3.4	31
21	The p-type conduction mechanism in Cu_2O: a first principles study. *Physical Chemistry Chemical Physics*, **2006**, 8, 5350-8	3.6	247
20	Ozone-Based Atomic Layer Deposition of Alumina from TMA: Growth, Morphology, and Reaction Mechanism. *Chemistry of Materials*, **2006**, 18, 3764-3773	9.6	143
19	Mechanism of the Verwey transition in magnetite: Jahn-Teller distortion and charge ordering patterns. *Journal of Physics Condensed Matter*, **2006**, 18, 10427-36	1.8	46
18	Predictive process design: a theoretical model of atomic layer deposition. *Computational Materials Science*, **2005**, 33, 20-25	3.2	25

17	Thermal decomposition mechanisms of hafnium and zirconium silicates at the atomic scale. *Journal of Applied Physics*, **2005**, 97, 114911	2.5	20
16	Simulating the structure and reactivity of oxide surfaces from first principles. *Theoretical and Computational Chemistry*, **2004**, 15, 297-324		1
15	Modelling the Deposition of High-k Dielectric Films by First Principles. *Journal of Electroceramics*, **2004**, 13, 117-120	1.5	18
14	Simulating the atomic layer deposition of alumina from first principles. *Journal of Materials Chemistry*, **2004**, 14, 3246		123
13	Ab initio study of □Al2O3 surfaces. *Physical Review B*, **2004**, 70,	3.3	159
12	Assignment of the (1□) surface of rutile TiO2(110) from first principles. *Physical Review B*, **2003**, 67,	3.3	21
11	Assigning the (1□) surface reconstruction on reduced rutile by first-principles energetics. *Physical Review B*, **2002**, 65,	3.3	17
10	First mixed valence cerium□organic trinuclear cluster [Ce3(OBut)10NO3] as a possible molecular switch: synthesis, structure and density functional calculations. *Dalton Transactions RSC*, **2002**, 1852-1856		15
9	A first principles survey of stoichiometric (1□) reconstructions on the rutile surface. *Surface Science*, **2001**, 495, 211-233	1.8	16
8	Energetically accessible reconstructions along interstitial rows onthe rutile (110) surface. *Physical Chemistry Chemical Physics*, **2001**, 3, 1954-1957	3.6	16
7	Auto-ionised products from the reaction of sodium clusters with dioxygen: Theory and experiment. *Physical Chemistry Chemical Physics*, **2000**, 2, 3415-3424	3.6	20
6	Electronic shell structure in monoxides and dioxides of sodium. *Physical Chemistry Chemical Physics*, **2000**, 2, 313-318	3.6	4
5	Clusters of aluminium, a density functional study. *Physical Chemistry Chemical Physics*, **1999**, 1, 13-21	3.6	158
4	Quantum chemistry: Large molecules □small computers. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 795-804		18
3	An ab initio study of the monoxides and dioxides of sodium. *Journal of Chemical Physics*, **1998**, 109, 4267-4280	3.9	19
2	New rigid backbone conjugated organic polymers with large fluorescence quantum yields. *Journal of the Chemical Society Chemical Communications*, **1995**, 1433		70
1	Models for ALD and MOCVD Growthof Rare Earth Oxides73-86		3