Simon D Elliott

List of Publications by Year
in descending order

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89 papers	3,583 citations	147566 31 h-index	143772 57 g-index
94 all docs	94 docs citations	94 times ranked	4469 citing authors

#	Article	IF	Citations
1	The p-type conduction mechanism in Cu2O: a first principles study. Physical Chemistry Chemical Physics, 2006, 8, 5350.	1.3	307
2	Ab initiostudy ofÎ³âˆ’Al2O3surfaces. Physical Review B, 2004, 70, .	1.1	197
3	Chiral Shells and Achiral Cores in CdS Quantum Dots. Nano Letters, 2008, 8, 2452-2457.	4.5	186
4	Clusters of aluminium, a density functional study. Physical Chemistry Chemical Physics, 1999, 1, 13-21.	1.3	173
5	Ozone-Based Atomic Layer Deposition of Alumina from TMA:Â Growth, Morphology, and Reaction Mechanism. Chemistry of Materials, 2006, 18, 3764-3773.	3.2	161
6	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
7	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:ms surface: Combined photoemission spectroscopy and density functional theory study. Physical Review B, 2008, 77, .	1.1	138
8	Simulating the atomic layer deposition of alumina from first principles. Journal of Materials Chemistry, 2004, 14, 3246.	6.7	134
9	Atomic-scale simulation of ALD chemistry. Semiconductor Science and Technology, 2012, 27, 074008.	1.0	90
10	New rigid backbone conjugated organic polymers with large fluorescence quantum yields. Journal of the Chemical Society Chemical Communications, 1995, , 1433.	2.0	74
11	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, .	0.9	74
12	Orientation of individual<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>molecules adsorbed on Cu(111): Low-temperature scanning tunneling microscopy and density functional calculations. Physical Review B, 2008, 77, .	1.1	73
13	Tuning the Transparency of Cu₂O with Substitutional Cation Doping. Chemistry of Materials, 2008, 20, 5522-5531.	3.2	67
14	Effect of Reaction Mechanism on Precursor Exposure Time in Atomic Layer Deposition of Silicon Oxide and Silicon Nitride. ACS Applied Materials & Interfaces, 2014, 6, 10534-10541.	4.0	65
15	Atomistic kinetic Monte Carlo study of atomic layer deposition derived from density functional theory. Journal of Computational Chemistry, 2014, 35, 244-259.	1.5	64
16	Modeling Mechanism and Growth Reactions for New Nanofabrication Processes by Atomic Layer Deposition. Advanced Materials, 2016, 28, 5367-5380.	11.1	60
17	Mechanism, Products, and Growth Rate of Atomic Layer Deposition of Noble Metals. Langmuir, 2010, 26, 9179-9182.	1.6	59
18	Cooperation between adsorbates accounts for the activation of atomic layer deposition reactions. Nanoscale, 2015, 7, 6311-6318.	2.8	54

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19	Role of Surface Termination in Atomic Layer Deposition of Silicon Nitride. Journal of Physical Chemistry Letters, 2015, 6, 3610-3614.	2.1	54
20	Mechanism of the Verwey transition in magnetite: Jahnâ€"Teller distortion and charge ordering patterns. Journal of Physics Condensed Matter, 2006, 18, 10427-10436.	0.7	53
21	First-Principles Modeling of the â€œClean-Upâ€• of Native Oxides during Atomic Layer Deposition onto IIIâ€"V Substrates. Journal of Physical Chemistry C, 2012, 116, 643-654.	1.5	50
22	Studying chemical vapor deposition processes with theoretical chemistry. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	50
23	Suppressing the Thermal and Ultraviolet Sensitivity of Kevlar by Infiltration and Hybridization with ZnO. Chemistry of Materials, 2017, 29, 10068-10074.	3.2	50
24	Deposition of Copper by Plasma-Enhanced Atomic Layer Deposition Using a Novel N-Heterocyclic Carbene Precursor. Chemistry of Materials, 2013, 25, 1132-1138.	3.2	46
25	Multiple Proton Diffusion and Film Densification in Atomic Layer Deposition Modeled by Density Functional Theory. Chemistry of Materials, 2013, 25, 878-889.	3.2	40
26	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.	3.2	39
27	Deposition of ZrO2 and HfO2 thin films by liquid injection MOCVD and ALD using ansa-metallocene zirconium and hafnium precursors. Journal of Materials Chemistry, 2008, 18, 4561.	6.7	38
28	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.	3.2	38
29	[illegible] hexagonal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi></mml:mrow></mml:math>-Si<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub [illegible]	1.1	35
30	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.	1.9	34
31	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, 8893-8901.	1.1	32
32	Mechanism for zirconium oxide atomic layer deposition using bis(methylcyclopentadienyl)methoxymethyl zirconium. Applied Physics Letters, 2007, 91, 253123.	1.5	31
33	Density Functional Theory Predictions of the Composition of Atomic Layer Deposition-Grown Ternary Oxides. ACS Applied Materials & Interfaces, 2013, 5, 3704-3715.	4.0	31
34	Tuning the electronic structure of the transparent conducting oxide Cu2O. Thin Solid Films, 2008, 516, 1468-1472.	0.8	30
35	Predictive process design: a theoretical model of atomic layer deposition. Computational Materials Science, 2005, 33, 20-25.	1.4	29
36	Competing Mechanisms in Atomic Layer Deposition of Er₂O₃ versus La₂O₃ from Cyclopentadienyl Precursors. Chemistry of Materials, 2010, 22, 117-129.	3.2	29

#	ARTICLE	IF	CITATIONS
37	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.	1.2	29
38	Improving ALD growth rate via ligand basicity: Quantum chemical calculations on lanthanum precursors. Surface and Coatings Technology, 2007, 201, 9076-9081.	2.2	28
39	TEMAZ/O3 atomic layer deposition process with doubled growth rate and optimized interface properties in metalâ€“insulatorâ€“metal capacitors. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2013, 31, 01A123.	0.9	25
40	Atomic scale model interfaces between high-khafnium silicates and silicon. Physical Review B, 2007, 75, .	1.1	24
41	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.	1.3	24
42	First-Principles Investigation of Câ€“H Bond Scission and Formation Reactions in Ethane, Ethene, and Ethyne Adsorbed on Ru(0001). Journal of Physical Chemistry C, 2014, 118, 26683-26694.	1.5	24
43	Quantum chemistry: Large molecules â€” small computers. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 795-804.	0.9	23
44	An ab initio study of the monoxides and dioxides of sodium. Journal of Chemical Physics, 1998, 109, 4267-4280.	1.2	23
45	Auto-ionised products from the reaction of sodium clusters with dioxygen: Theory and experiment. Physical Chemistry Chemical Physics, 2000, 2, 3415-3424.	1.3	23
46	A first principles survey of stoichiometric (1Ã—2) reconstructions on the rutile surface. Surface Science, 2001, 495, 211-233.	0.8	23
47	Assignment of the(1Ã—2)surface of rutileTiO2(110)from first principles. Physical Review B, 2003, 67, .	1.1	23
48	Thermal Stability of Precursors for Atomic Layer Deposition of TiO₂, ZrO₂, and HfO₂: An Ab Initio Study of Î±-Hydrogen Abstraction in Bis-cyclopentadienyl Dimethyl Complexes. Journal of Physical Chemistry A, 2010, 114, 1879-1886.	1.1	23
49	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.	4.0	23
50	Thermal decomposition mechanisms of hafnium and zirconium silicates at the atomic scale. Journal of Applied Physics, 2005, 97, 114911.	1.1	22
51	Modelling the Deposition of High-k Dielectric Films by First Principles. Journal of Electroceramics, 2004, 13, 117-120.	0.8	20
52	(Invited) Reaction Mechanisms in ALD of Ternary Oxides. ECS Transactions, 2011, 41, 175-183.	0.3	20
53	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
54	First mixed valence ceriumâ€“organic trinuclear cluster [Ce3(OBut)10NO3] as a possible molecular switch: synthesis, structure and density functional calculations. Dalton Transactions RSC, 2002, , 1852-1856.	2.3	19

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55	Assigning the(1Ã—2)surface reconstruction on reduced rutile by first-principles energetics. Physical Review B, 2002, 65, .	1.1	18
56	TiCp*(OMe)₃ versus Ti(OMe)₄ in Atomic Layer Deposition of TiO₂ with Waterâ€”<I>Ab Initio</I> Modelling of Atomic Layer Deposition Surface Reactions. Journal of Nanoscience and Nanotechnology, 2011, 11, 8089-8093.	0.9	18
57	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.	3.2	17
58	Copper reduction and atomic layer deposition by oxidative decomposition of formate by hydrazine. RSC Advances, 2014, 4, 34448-34453.	1.7	17
59	Kinetic Monte Carlo Study of the Atomic Layer Deposition of Zinc Oxide. Journal of Physical Chemistry C, 2018, 122, 27044-27058.	1.5	17
60	Energetically accessible reconstructions along interstitial rows on the rutile (110) surface. Physical Chemistry Chemical Physics, 2001, 3, 1954-1957.	1.3	16
61	Decomposition of Metal Alkylamides, Alkyls, and Halides at Reducible Oxide Surfaces: Mechanism of â€˜Clean-upâ€™ During Atomic Layer Deposition of Dielectrics onto IIIâ€“V Substrates. Chemistry of Materials, 2014, 26, 2427-2437.	3.2	16
62	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.	1.5	16
63	Optical and microstructural properties of p-type SrCu2O2: First principles modeling and experimental studies. Thin Solid Films, 2007, 515, 8624-8631.	0.8	15
64	First-principles study of oxygen and aluminum defects in Î²-Si3N4: Compensation and charge trapping. Computational Materials Science, 2014, 81, 178-183.	1.4	14
65	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.	1.5	14
66	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.	3.2	14
67	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
68	Modeling of Precursors for Atomic Layer Deposition of Magnesium and Calcium Oxide. Chemical Vapor Deposition, 2013, 19, 117-124.	1.4	12
69	Investigating routes toward atomic layer deposition of silicon carbide: <i>Ab initio</i> screening of potential silicon and carbon precursors. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2017, 35, .	0.9	11
70	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.	3.2	11
71	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.	0.5	10
72	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.	1.5	8

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73	Prediction and Validation of the Process Window for Atomic Layer Etching: HF Exposure on TiO₂. Journal of Physical Chemistry C, 2021, 125, 25589-25599.	1.5	8
74	Quantum chemical and solution phase evaluation of metallocenes as reducing agents for the prospective atomic layer deposition of copper. Dalton Transactions, 2015, 44, 10188-10199.	1.6	7
75	The role of local chemical hardness and van der Waals interactions in the anionic polymerization of alkyl cyanoacrylates. Polymer Chemistry, 2016, 7, 3236-3243.	1.9	7
76	Electronic shell structure in monoxides and dioxides of sodium. Physical Chemistry Chemical Physics, 2000, 2, 313-318.	1.3	6
77	Reductive Elimination of Hypersilyl Halides from Zinc(II) Complexes. Implications for Electropositive Metal Thin Film Growth. Inorganic Chemistry, 2015, 54, 7-9.	1.9	6
78	Non-stoichiometric oxide and metal interfaces and reactions. Applied Physics A: Materials Science and Processing, 2009, 96, 543-548.	1.1	5
79	Understanding 'Clean-Up' of IIIâ€“V Native Oxides During Atomic Layer Deposition Using Bulk First Principles Models. Journal of Nanoscience and Nanotechnology, 2011, 11, 8246-8250.	0.9	5
80	Models for ALD and MOCVD Growthof Rare Earth Oxides. , 0, , 73-86.		4
81	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.	0.9	4
82	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.	1.5	3
83	Combining Experimental and DFT Investigation of the Mechanism Involved in Thermal Etching of Titanium Nitride Using Alternate Exposures of NbF 5 and CCl 4 , or CCl 4 Only. Advanced Materials Interfaces, 2021, 8, 2101085.	1.9	3
84	An Ab Initio Evaluation of Cyclopentadienyl Precursors for the Atomic Layer Deposition of Hafnia and Zirconia. ECS Transactions, 2007, 11, 113-121.	0.3	2
85	Stress in silicon interlayers at the SiOxâˆ•Ge interface. Applied Physics Letters, 2007, 90, 143511.	1.5	2
86	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.	3.2	2
87	ALD Simulations. , 2014, , 47-69.		2
88	Simulating the structure and reactivity of oxide surfaces from first principles. Theoretical and Computational Chemistry, 2004, 15, 297-324.	0.2	1
89	Selected Peer-Reviewed Articles from The EuroCVD-18 Conference (EuroCVD 2011). Journal of Nanoscience and Nanotechnology, 2011, 11, 7945-7947.	0.9	0