Simon D Elliott

List of Publications by Citations

Source: https://exaly.com/author-pdf/274337/simon-d-elliott-publications-by-citations.pdf
Version: 2024-04-26

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
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	The p-type conduction mechanism in Cu2O: a first principles study. *Physical Chemistry Chemical Physics*, **2006**, 8, 5350-8	3.6	247
87	Chiral shells and achiral cores in CdS quantum dots. *Nano Letters*, **2008**, 8, 2452-7	11.5	159
86	Ab initio study of ▯Al2O3 surfaces. *Physical Review B*, **2004**, 70,	3.3	159
85	Clusters of aluminium, a density functional study. *Physical Chemistry Chemical Physics*, **1999**, 1, 13-21	3.6	158
84	Ozone-Based Atomic Layer Deposition of Alumina from TMA: Growth, Morphology, and Reaction Mechanism. *Chemistry of Materials*, **2006**, 18, 3764-3773	9.6	143
83	Simulating the atomic layer deposition of alumina from first principles. *Journal of Materials Chemistry*, **2004**, 14, 3246		123
82	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
81	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
80	Atomic-scale simulation of ALD chemistry. *Semiconductor Science and Technology*, **2012**, 27, 074008	1.8	72
79	New rigid backbone conjugated organic polymers with large fluorescence quantum yields. *Journal of the Chemical Society Chemical Communications*, **1995**, 1433		70
78	Orientation of individual C60 molecules adsorbed on Cu(111): Low-temperature scanning tunneling microscopy and density functional calculations. *Physical Review B*, **2008**, 77,	3.3	66
77	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
76	Tuning the Transparency of Cu2O with Substitutional Cation Doping. *Chemistry of Materials*, **2008**, 20, 5522-5531	9.6	56
75	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
74	Mechanism, products, and growth rate of atomic layer deposition of noble metals. *Langmuir*, **2010**, 26, 9179-82	4	50
73	Modeling Mechanism and Growth Reactions for New Nanofabrication Processes by Atomic Layer Deposition. *Advanced Materials*, **2016**, 28, 5367-80	24	48
72	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

71	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
70	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
69	Cooperation between adsorbates accounts for the activation of atomic layer deposition reactions. *Nanoscale*, **2015**, 7, 6311-8	7.7	43
68	Role of Surface Termination in Atomic Layer Deposition of Silicon Nitride. *Journal of Physical Chemistry Letters*, **2015**, 6, 3610-4	6.4	40
67	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
66	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
65	Studying chemical vapor deposition processes with theoretical chemistry. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	36
64	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
63	Suppressing the Thermal and Ultraviolet Sensitivity of Kevlar by Infiltration and Hybridization with ZnO. *Chemistry of Materials*, **2017**, 29, 10068-10074	9.6	32
62	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
61	Mechanism for zirconium oxide atomic layer deposition using bis(methylcyclopentadienyl)methoxymethyl zirconium. *Applied Physics Letters*, **2007**, 91, 253123	3.4	31
60	Native defects in hexagonal β-Si_3N_4 studied using density functional theory calculations. *Physical Review B*, **2011**, 83,	3.3	30
59	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
58	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
57	Tuning the electronic structure of the transparent conducting oxide Cu_2O. *Thin Solid Films*, **2008**, 516, 1468-1472	2.2	29
56	Improving ALD growth rate via ligand basicity: Quantum chemical calculations on lanthanum precursors. *Surface and Coatings Technology*, **2007**, 201, 9076-9081	4.4	27
55	Competing Mechanisms in Atomic Layer Deposition of Er_2O_3 versus La_2O_3 from Cyclopentadienyl Precursors. *Chemistry of Materials*, **2010**, 22, 117-129	9.6	26
54	Predictive process design: a theoretical model of atomic layer deposition. *Computational Materials Science*, **2005**, 33, 20-25	3.2	25

53	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
52	Atomic scale model interfaces between high-k hafnium silicates and silicon. *Physical Review B*, **2007**, 75,	3.3	23
51	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
50	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
49	Assignment of the (1□) surface of rutile TiO2(110) from first principles. *Physical Review B*, **2003**, 67,	3.3	21
48	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
47	Thermal decomposition mechanisms of hafnium and zirconium silicates at the atomic scale. *Journal of Applied Physics*, **2005**, 97, 114911	2.5	20
46	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
45	An ab initio study of the monoxides and dioxides of sodium. *Journal of Chemical Physics*, **1998**, 109, 4267-4280	3.9	19
44	Quantum chemistry: Large molecules □small computers. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 795-804		18
43	Modelling the Deposition of High-k Dielectric Films by First Principles. *Journal of Electroceramics*, **2004**, 13, 117-120	1.5	18
42	TEMAZ/O3 atomic layer deposition process with doubled growth rate and optimized interface properties in metal□nsulator□metal capacitors. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2013**, 31, 01A123	2.9	17
41	Assigning the (1□) surface reconstruction on reduced rutile by first-principles energetics. *Physical Review B*, **2002**, 65,	3.3	17
40	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
39	A first principles survey of stoichiometric (1□) reconstructions on the rutile surface. *Surface Science*, **2001**, 495, 211-233	1.8	16
38	Energetically accessible reconstructions along interstitial rows onthe rutile (110) surface. *Physical Chemistry Chemical Physics*, **2001**, 3, 1954-1957	3.6	16
37	Decomposition of Metal Alkylamides, Alkyls, and Halides at Reducible Oxide Surfaces: Mechanism of □Clean-up□During Atomic Layer Deposition of Dielectrics onto III□ Substrates. *Chemistry of Materials*, **2014**, 26, 2427-2437	9.6	15
36	Copper reduction and atomic layer deposition by oxidative decomposition of formate by hydrazine. *RSC Advances*, **2014**, 4, 34448-34453	3.7	15

35	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
34	Optical and microstructural properties of p-type SrCu2O2: First principles modeling and experimental studies. *Thin Solid Films*, **2007**, 515, 8624-8631	2.2	15
33	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
32	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
31	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
30	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
29	(Invited) Reaction Mechanisms in ALD of Ternary Oxides. *ECS Transactions*, **2011**, 41, 175-183	1	14
28	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
27	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
26	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
25	First-principles study of oxygen and aluminum defects in □Si3N4: Compensation and charge trapping. *Computational Materials Science*, **2014**, 81, 178-183	3.2	11
24	Kinetic Monte Carlo Study of the Atomic Layer Deposition of Zinc Oxide. *Journal of Physical Chemistry C*, **2018**, 122, 27044-27058	3.8	11
23	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
22	Modeling of Precursors for Atomic Layer Deposition of Magnesium and Calcium Oxide. *Chemical Vapor Deposition*, **2013**, 19, 117-124		10
21	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
20	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
19	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
18	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

17	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
16	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
15	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
14	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
13	Non-stoichiometric oxide and metal interfaces and reactions. *Applied Physics A: Materials Science and Processing*, **2009**, 96, 543-548	2.6	4
12	Electronic shell structure in monoxides and dioxides of sodium. *Physical Chemistry Chemical Physics*, **2000**, 2, 313-318	3.6	4
11	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
10	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
9	Models for ALD and MOCVD Growthof Rare Earth Oxides73-86		3
8	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
7	An Ab Initio Evaluation of Cyclopentadienyl Precursors for the Atomic Layer Deposition of Hafnia and Zirconia. *ECS Transactions*, **2007**, 11, 113-121	1	2
6	Stress in silicon interlayers at the SiOx/Ge interface. *Applied Physics Letters*, **2007**, 90, 143511	3.4	2
5	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
4	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
3	ALD Simulations **2014**, 47-69		2
2	Simulating the structure and reactivity of oxide surfaces from first principles. *Theoretical and Computational Chemistry*, **2004**, 15, 297-324		1
1	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