Mathew D Halls

List of Publications by Year
in descending order

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85	5,381	159585	82547
papers	citations	30 h-index	72 g-index

88	88	88	7919
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Design and Synthesis of Novel Oxime Ester Photoinitiators Augmented by Automated Machine Learning. Chemistry of Materials, 2022, 34, 116-127.	6.7	13
2	Organic radical emitters: nature of doublet excitons in emissive layers. Physical Chemistry Chemical Physics, 2022, 24, 16891-16899.	2.8	7
3	66â€3: Active Learning for the Design of Novel OLED Materials. Digest of Technical Papers SID International Symposium, 2022, 53, 885-888.	0.3	3
4	Pâ€130: Organic Thin Films for OLED Applications: Simulating the Influence of Deposition Conditions and Substrate. Digest of Technical Papers SID International Symposium, 2022, 53, 1499-1502.	0.3	0
5	Characterizing moisture uptake and plasticization effects of water on amorphous amylose starch models using molecular dynamics methods. Carbohydrate Polymers, 2021, 252, 117161.	10.2	9
6	High-Throughput Molecular Dynamics Simulations and Validation of Thermophysical Properties of Polymers for Various Applications. ACS Applied Polymer Materials, 2021, 3, 620-630.	4.4	35
7	Highly efficient implementation of the analytical gradients of pseudospectral time-dependent density functional theory. Journal of Chemical Physics, 2021, 155, 024115.	3.0	2
8	Generative machine learning for accelerated discovery of OLED materials. , 2021, , .		0
9	Enhancing OLED outcoupling efficiency via atomistic-scale simulations. , 2021, , .		1
10	Pseudospectral implementations of <scp>longâ€range</scp> corrected density functional theory. Journal of Computational Chemistry, 2021, 42, 2089-2102.	3.3	10
11	Accelerated design and optimization of novel OLED materials via active learning. , 2021, , .		2
12	De Novo Design of Molecules with Low Hole Reorganization Energy Based on a Quarter-Million Molecule DFT Screen. Journal of Physical Chemistry A, 2021, 125, 7331-7343.	2.5	12
13	Active Learning Accelerates Design and Optimization of Hole-Transporting Materials for Organic Electronics. Frontiers in Chemistry, 2021, 9, 800371.	3.6	11
14	Design of Organic Electronic Materials With a Goal-Directed Generative Model Powered by Deep Neural Networks and High-Throughput Molecular Simulations. Frontiers in Chemistry, 2021, 9, 800370.	3.6	12
15	Microplastics Outreach Program: A Systems-Thinking Approach To Teach High School Students about the Chemistry and Impacts of Plastics. Journal of Chemical Education, 2020, 97, 137-142.	2.3	13
16	Estimation of electron and hole mobility of 50 homogeneous fullerene amorphous structures (C60,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 2020, 78, 105571.	2.6	10
17	Molecular Design Based on Donor-Weak Donor Scaffold for Blue Thermally-Activated Delayed Fluorescence Designed by Combinatorial DFT Calculations. Frontiers in Chemistry, 2020, 8, 403.	3.6	18
18	Massive Theoretical Screen of Hole Conducting Organic Materials in the Heteroacene Family by Using a Cloud-Computing Environment. Journal of Physical Chemistry A, 2020, 124, 1981-1992.	2.5	10

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19	Using Molecular Simulation with High-temperature Composites Resins. , 2019, , .		1
20	Chemical Modification Mechanisms in Hybrid Hafnium Oxo-methacrylate Nanocluster Photoresists for Extreme Ultraviolet Patterning. Chemistry of Materials, 2018, 30, 6192-6206.	6.7	31
21	Atomistic simulations of mechanical and thermophysical properties of OLED materials. , 2018, , .		2
22	Automated Transition State Search and Its Application to Diverse Types of Organic Reactions. Journal of Chemical Theory and Computation, 2017, 13, 5780-5797.	5.3	125
23	Atomic layer deposition of boron-containing films using B2F4. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2016, 34, .	2.1	8
24	Accelerated discovery of OLED materials through atomic-scale simulation. Proceedings of SPIE, 2016, , .	0.8	3
25	In silico evaluation of highly efficient organic light-emitting materials. , 2016, , .		1
26	Highly efficient implementation of pseudospectral timeâ€dependent densityâ€functional theory for the calculation of excitation energies of large molecules. Journal of Computational Chemistry, 2016, 37, 1425-1441.	3.3	29
27	Surface etching, chemical modification and characterization of silicon nitride and silicon oxideâ€"selective functionalization of Si₃N₄and SiO₂. Journal of Physics Condensed Matter, 2016, 28, 094014.	1.8	31
28	Estimation of charge carrier mobility in amorphous organic materials using percolation corrected random-walk model. Organic Electronics, 2016, 29, 50-56.	2.6	42
29	Quantum Mechanical Simulation for the Analysis, Optimization and Accelerated Development of Precursors and Processes for Atomic Layer Deposition (ALD). Journal of the Korean Ceramic Society, 2016, 53, 317-324.	2.3	11
30	Optical simulations for fractional fluorine terminated coatings on nanoimprint lithography masks. , 2015, , .		0
31	Ethylenediamine Grafting on Oxide-Free H-, 1/3 ML F-, and Cl-Terminated Si(111) Surfaces. Chemistry of Materials, 2015, 27, 6268-6281.	6.7	26
32	Discovery of New Anode SEI Forming Additives Using an in silico Evolutionary Approach. ECS Transactions, 2015, 69, 67-74.	0.5	5
33	Chemical Nature and Control of High-k Dielectric/III-V Interfaces. ECS Transactions, 2015, 66, 65-76.	0.5	1
34	Atomic layer deposition of dopants for recoil implantation in finFET sidewalls. , 2014, , .		1
35	Fluorine coatings for nanoimprint lithography masks. , 2014, , .		0
36	Virtual screening for OLED materials. Proceedings of SPIE, 2014, , .	0.8	3

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37	Role of Interfacial Aluminum Silicate and Silicon as Barrier Layers for Atomic Layer Deposition of Al₂O₃ Films on Chemically Cleaned InP(100) Surfaces. Journal of Physical Chemistry C, 2014, 118, 29164-29179.	3.1	5
38	Surface Oxide Characterization and Interface Evolution in Atomic Layer Deposition of Al₂O₃ on InP(100) Studied by in Situ Infrared Spectroscopy. Journal of Physical Chemistry C, 2014, 118, 5862-5871.	3.1	16
39	High-throughput quantum chemistry and virtual screening for OLED material components. Proceedings of SPIE, 2013, , .	0.8	7
40	Virtual screening of electron acceptor materials for organic photovoltaic applications. New Journal of Physics, 2013, 15, 105029.	2.9	24
41	Jaguar: A highâ€performance quantum chemistry software program with strengths in life and materials sciences. International Journal of Quantum Chemistry, 2013, 113, 2110-2142.	2.0	1,426
42	Substrate Selectivity of (^tBu-Allyl)Co(CO)₃ during Thermal Atomic Layer Deposition of Cobalt. Chemistry of Materials, 2012, 24, 1025-1030.	6.7	57
43	Atomistic Simulations of Microelectronic Materials: Prediction of Mechanical, Thermal, and Electrical Properties. , 2012, , 3-24.		0
44	Nature of Hydrophilic Aluminum Fluoride and Oxyaluminum Fluoride Surfaces Resulting from XeF₂ Treatment of Al and Al₂O₃. Journal of Physical Chemistry C, 2011, 115, 21351-21357.	3.1	31
45	High-throughput quantum chemistry and virtual screening for lithium ion battery electrolyte additives. Journal of Power Sources, 2010, 195, 1472-1478.	7.8	89
46	XeF2-induced removal of SiO2 near Si surfaces at 300 K: An unexpected proximity effect.. Journal of Applied Physics, 2010, 108, 114914.	2.5	17
47	Suppression of substrate oxidation during ozone based atomic layer deposition of Al2O3: Effect of ozone flow rate. Applied Physics Letters, 2010, 97, 162903.	3.3	20
48	A Family of Heteroleptic Titanium Guanidinates: Synthesis, Thermolysis, and Surface Reactivity. Inorganic Chemistry, 2010, 49, 1976-1982.	4.0	24
49	Computational materials engineering: Capabilities of atomic-scale prediction of mechanical, thermal, and electrical properties of microelectronic materials. , 2010, , .		1
50	Surface and Interface Processes during Atomic Layer Deposition of Copper on Silicon Oxide. Langmuir, 2010, 26, 3911-3917.	3.5	73
51	FTIR study of copper agglomeration during atomic layer deposition of copper. Materials Research Society Symposia Proceedings, 2009, 1155, 1.	0.1	4
52	Nitrogen interaction with hydrogen-terminated silicon surfaces at the atomic scale. Nature Materials, 2009, 8, 825-830.	27.5	57
53	In Situ Infrared Characterization during Atomic Layer Deposition of Lanthanum Oxide. Journal of Physical Chemistry C, 2009, 113, 654-660.	3.1	80
54	Density functional theory study of Al₂₃, Al₂₆and Al₉₂clusters. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 125103.	1.5	9

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55	Chemical Properties of Oxidized Silicon Carbide Surfaces upon Etching in Hydrofluoric Acid. Journal of the American Chemical Society, 2009, 131, 16808-16813.	13.7	124
56	Detection of a Formate Surface Intermediate in the Atomic Layer Deposition of High-Îº Dielectrics Using Ozone. Chemistry of Materials, 2008, 20, 3248-3250.	6.7	58
57	Chemical failure modes of AlQ3-based OLEDs: AlQ3 hydrolysis. Physical Chemistry Chemical Physics, 2006, 8, 1371.	2.8	63
58	Hydrogen-Bonding Interactions in Peptide Nucleic Acid and Deoxyribonucleic Acid:â€‰ A Comparative Study. Journal of Physical Chemistry B, 2006, 110, 3336-3343.	2.6	20
59	Guest Species/Discrete Carbon Nanotube Inner Phase Charge Transfer and Externallonization. Journal of Computational and Theoretical Nanoscience, 2006, 3, 398-404.	0.4	2
60	Carbon Nanotube Inner Phase Chemistry:Â The Cl-Exchange SN2 Reaction. Nano Letters, 2005, 5, 1861-1866.	9.1	31
61	Chlorination of hydrogen-terminated silicon (111) surfaces. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2005, 23, 1100-1106.	2.1	71
62	Hafnium Oxide and Zirconium Oxide Atomic Layer Deposition:â€‰ Initial Precursor and Potential Side-Reaction Product Pathways with H/Si(100)-2Ã—1. Journal of Physical Chemistry B, 2005, 109, 4969-4976.	2.6	11
63	Probing Occupied States of the Molecular Layer in Auâˆ'Alkanedithiolâˆ'GaAs Diodes. Journal of Physical Chemistry B, 2005, 109, 5719-5723.	2.6	24
64	Raman scattering of complex sodium aluminum hydride for hydrogen storage. Chemical Physics Letters, 2004, 388, 430-435.	2.6	20
65	Quantum chemical studies of semiconductor surface chemistry using cluster models. Molecular Physics, 2004, 102, 381-393.	1.7	43
66	Importance of Steric Effects in Cluster Models of Silicon Surface Chemistry:Â ONIOM Studies of the Atomic Layer Deposition (ALD) of Al2O3on H/Si(111)â€. Journal of Physical Chemistry A, 2004, 108, 2982-2987.	2.5	29
67	Atomic Layer Deposition Growth Reactions of Al2O3 on Si(100)-2Ã—1. Journal of Physical Chemistry B, 2004, 108, 4058-4062.	2.6	60
68	Infrared Intensities of Î½(Siâˆ'H) on H/Si(100)-2Ã—1:Â Effect of O Incorporation and Agglomeration. Journal of Physical Chemistry B, 2004, 108, 19388-19391.	2.6	17
69	Water Alignment and Proton Conduction inside Carbon Nanotubes. Physical Review Letters, 2003, 90, 195503.	7.8	237
70	Atomic layer deposition ofAl2O3on H-passivated Si:â€ƒAl(CH3)2OHsurface reactions withH/Si(100)â€“2Ã—1. Physical Review B, 2003, 68, .	3.2	41
71	Atomic layer deposition of Al2O3 on H-passivated Si. I. Initial surface reaction pathways with H/Si(100)-2Ã—1. Journal of Chemical Physics, 2003, 118, 10221-10226.	3.0	51
72	Ab initio simulations of oxygen atom insertion and substitutional doping of carbon nanotubes. Journal of Chemical Physics, 2002, 116, 9014-9020.	3.0	41

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73	Direct Dynamics Studies of CO-Assisted Carbon Nanotube Growth. Journal of Physical Chemistry B, 2002, 106, 12418-12425.	2.6	16
74	Chemistry Inside Carbon Nanotubes:Â the Menshutkin SN2 Reaction. Journal of Physical Chemistry B, 2002, 106, 1921-1925.	2.6	131
75	Ring-opening of the cyclopropyl radical in the condensed phase: A combined density functional theory/molecular mechanics quasiclassical trajectory study. Physical Chemistry Chemical Physics, 2002, 4, 5066-5071.	2.8	11
76	Noncovalent Engineering of Carbon Nanotube Surfaces by Rigid, Functional Conjugated Polymers. Journal of the American Chemical Society, 2002, 124, 9034-9035.	13.7	765
77	Molecular Orbital Study of the First Excited State of the OLED Material Tris(8-hydroxyquinoline)aluminum(III). Chemistry of Materials, 2001, 13, 2632-2640.	6.7	221
78	Structure and infrared (IR) assignments for the OLED material: N,Nâ€²-diphenyl-N,Nâ€²-bis(1-naphthyl)-1,1â€²-biphenyl-4,4â€³-diamine (NPB). Physical Chemistry Chemical Physics, 2001, 3, 2131-2136.	2.8	60
79	Harmonic frequency scaling factors for Hartree-Fock, S-VWN, B-LYP, B3-LYP, B3-PW91 and MP2 with the Sadlej pVTZ electric property basis set. Theoretical Chemistry Accounts, 2001, 105, 413-421.	1.4	411
80	Ab initio calculation of the Îε interaction potential and vibrational levels of. Chemical Physics Letters, 2001, 339, 427-432.	2.6	27
81	Comparison study of the prediction of Raman intensities using electronic structure methods. Journal of Chemical Physics, 1999, 111, 8819-8824.	3.0	137
82	Vibrational spectra of halophthalonitriles. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 54, 305-317.	3.9	13
83	Comparison of the performance of local, gradient-corrected, and hybrid density functional models in predicting infrared intensities. Journal of Chemical Physics, 1998, 109, 10587-10593.	3.0	163
84	Vibrational spectra and structure of tris(8-hydroÃ—yquinoline)aluminum(III). Canadian Journal of Chemistry, 1998, 76, 1730-1736.	1.1	51
85	Machine Learning for the Design of Novel OLED Materials. ACS Symposium Series, 0, , 33-49.	0.5	2