Mathew D Halls

List of Publications by Year
in descending order

85 papers	5,381 citations	159585 30 h-index	82547 72 g-index
88 all docs	88 docs citations	88 times ranked	7919 citing authors

#	Article	IF	Citations
1	Jaguar: A high‑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
2	Noncovalent Engineering of Carbon Nanotube Surfaces by Rigid, Functional Conjugated Polymers. Journal of the American Chemical Society, 2002, 124, 9034-9035.	13.7	765
3	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
4	Water Alignment and Proton Conduction inside Carbon Nanotubes. Physical Review Letters, 2003, 90, 195503.	7.8	237
5	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
6	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
7	Comparison study of the prediction of Raman intensities using electronic structure methods. Journal of Chemical Physics, 1999, 111, 8819-8824.	3.0	137
8	Chemistry Inside Carbon Nanotubes: the Menshutkin SN2 Reaction. Journal of Physical Chemistry B, 2002, 106, 1921-1925.	2.6	131
9	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
10	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
11	High-throughput quantum chemistry and virtual screening for lithium ion battery electrolyte additives. Journal of Power Sources, 2010, 195, 1472-1478.	7.8	89
12	In Situ Infrared Characterization during Atomic Layer Deposition of Lanthanum Oxide. Journal of Physical Chemistry C, 2009, 113, 654-660.	3.1	80
13	Surface and Interface Processes during Atomic Layer Deposition of Copper on Silicon Oxide. Langmuir, 2010, 26, 3911-3917.	3.5	73
14	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
15	Chemical failure modes of AlQ3-based OLEDs: AlQ3 hydrolysis. Physical Chemistry Chemical Physics, 2006, 8, 1371.	2.8	63
16	Structure and infrared (IR) assignments for the OLED material: N,N′-diphenyl-N,N′-bis(1-naphthyl)-1,1′-biphenyl-4,4‴-diamine (NPB). Physical Chemistry Chemical Physics, 2001, 3, 2131-2136.	2.8	60
17	Atomic Layer Deposition Growth Reactions of Al2O3 on Si(100)-2×1. Journal of Physical Chemistry B, 2004, 108, 4058-4062.	2.6	60
18	Detection of a Formate Surface Intermediate in the Atomic Layer Deposition of High-κ Dielectrics Using Ozone. Chemistry of Materials, 2008, 20, 3248-3250.	6.7	58

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19	Nitrogen interaction with hydrogen-terminated silicon surfaces at the atomic scale. Nature Materials, 2009, 8, 825-830.	27.5	57
20	Substrate Selectivity of (^{t}Bu-Allyl)Co(CO)$_3$ during Thermal Atomic Layer Deposition of Cobalt. Chemistry of Materials, 2012, 24, 1025-1030.	6.7	57
21	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
22	Vibrational spectra and structure of tris(8-hydroÃ—yquinoline)aluminum(III). Canadian Journal of Chemistry, 1998, 76, 1730-1736.	1.1	51
23	Quantum chemical studies of semiconductor surface chemistry using cluster models. Molecular Physics, 2004, 102, 381-393.	1.7	43
24	Estimation of charge carrier mobility in amorphous organic materials using percolation corrected random-walk model. Organic Electronics, 2016, 29, 50-56.	2.6	42
25	Ab initio simulations of oxygen atom insertion and substitutional doping of carbon nanotubes. Journal of Chemical Physics, 2002, 116, 9014-9020.	3.0	41
26	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
27	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
28	Carbon Nanotube Inner Phase Chemistry:Â The Cl-Exchange SN2 Reaction. Nano Letters, 2005, 5, 1861-1866.	9.1	31
29	Nature of Hydrophilic Aluminum Fluoride and Oxyaluminum Fluoride Surfaces Resulting from XeF$_2$ Treatment of Al and Al$_2$O$_3$. Journal of Physical Chemistry C, 2011, 115, 21351-21357.	3.1	31
30	Surface etching, chemical modification and characterization of silicon nitride and silicon oxideâ€"selective functionalization of Si$_3$N$_4$and SiO$_2$. Journal of Physics Condensed Matter, 2016, 28, 094014.	1.8	31
31	Chemical Modification Mechanisms in Hybrid Hafnium Oxo-methacrylate Nanocluster Photoresists for Extreme Ultraviolet Patterning. Chemistry of Materials, 2018, 30, 6192-6206.	6.7	31
32	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
33	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
34	Ab initio calculation of the Î£ interaction potential and vibrational levels of. Chemical Physics Letters, 2001, 339, 427-432.	2.6	27
35	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
36	Probing Occupied States of the Molecular Layer in Auˆ'Alkanedithiolˆ'GaAs Diodes. Journal of Physical Chemistry B, 2005, 109, 5719-5723.	2.6	24

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37	A Family of Heteroleptic Titanium Guanidinates: Synthesis, Thermolysis, and Surface Reactivity. Inorganic Chemistry, 2010, 49, 1976-1982.	4.0	24
38	Virtual screening of electron acceptor materials for organic photovoltaic applications. New Journal of Physics, 2013, 15, 105029.	2.9	24
39	Raman scattering of complex sodium aluminum hydride for hydrogen storage. Chemical Physics Letters, 2004, 388, 430-435.	2.6	20
40	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
41	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
42	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
43	Infrared Intensities of Î½(Siâˆ¼H) 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
44	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
45	Direct Dynamics Studies of CO-Assisted Carbon Nanotube Growth. Journal of Physical Chemistry B, 2002, 106, 12418-12425.	2.6	16
46	Surface Oxide Characterization and Interface Evolution in Atomic Layer Deposition of Al$_2$O$_3$ on InP(100) Studied by in Situ Infrared Spectroscopy. Journal of Physical Chemistry C, 2014, 118, 5862-5871.	3.1	16
47	Vibrational spectra of halophthalonitriles. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 54, 305-317.	3.9	13
48	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
49	Design and Synthesis of Novel Oxime Ester Photoinitiators Augmented by Automated Machine Learning. Chemistry of Materials, 2022, 34, 116-127.	6.7	13
50	*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
51	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
52	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
53	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
54	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

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55	Active Learning Accelerates Design and Optimization of Hole-Transporting Materials for Organic Electronics. Frontiers in Chemistry, 2021, 9, 800371.	3.6	11
56	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
57	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
58	Pseudospectral implementations of <scp>long‐range</scp> corrected density functional theory. Journal of Computational Chemistry, 2021, 42, 2089-2102.	3.3	10
59	Density functional theory study of Al_{23}, Al_{26} and Al_{92} clusters. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 125103.	1.5	9
60	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
61	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
62	High-throughput quantum chemistry and virtual screening for OLED material components. Proceedings of SPIE, 2013, , .	0.8	7
63	Organic radical emitters: nature of doublet excitons in emissive layers. Physical Chemistry Chemical Physics, 2022, 24, 16891-16899.	2.8	7
64	Role of Interfacial Aluminum Silicate and Silicon as Barrier Layers for Atomic Layer Deposition of Al_2O_3 Films on Chemically Cleaned InP(100) Surfaces. Journal of Physical Chemistry C, 2014, 118, 29164-29179.	3.1	5
65	Discovery of New Anode SEI Forming Additives Using an in silico Evolutionary Approach. ECS Transactions, 2015, 69, 67-74.	0.5	5
66	FTIR study of copper agglomeration during atomic layer deposition of copper. Materials Research Society Symposia Proceedings, 2009, 1155, 1.	0.1	4
67	Virtual screening for OLED materials. Proceedings of SPIE, 2014, , .	0.8	3
68	Accelerated discovery of OLED materials through atomic-scale simulation. Proceedings of SPIE, 2016, , .	0.8	3
69	66‐3: Active Learning for the Design of Novel OLED Materials. Digest of Technical Papers SID International Symposium, 2022, 53, 885-888.	0.3	3
70	Highly efficient implementation of the analytical gradients of pseudospectral time-dependent density functional theory. Journal of Chemical Physics, 2021, 155, 024115.	3.0	2
71	Accelerated design and optimization of novel OLED materials via active learning. , 2021, , .		2
72	Guest Species/Discrete Carbon Nanotube Inner Phase Charge Transfer and ExternalIonization. Journal of Computational and Theoretical Nanoscience, 2006, 3, 398-404.	0.4	2

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73	Atomistic simulations of mechanical and thermophysical properties of OLED materials. , 2018, , .		2
74	Machine Learning for the Design of Novel OLED Materials. ACS Symposium Series, 0, , 33-49.	0.5	2
75	Computational materials engineering: Capabilities of atomic-scale prediction of mechanical, thermal, and electrical properties of microelectronic materials. , 2010, , .		1
76	Atomic layer deposition of dopants for recoil implantation in finFET sidewalls. , 2014, , .		1
77	Chemical Nature and Control of High-k Dielectric/III-V Interfaces. ECS Transactions, 2015, 66, 65-76.	0.5	1
78	In silico evaluation of highly efficient organic light-emitting materials. , 2016, , .		1
79	Enhancing OLED outcoupling efficiency via atomistic-scale simulations. , 2021, , .		1
80	Using Molecular Simulation with High-temperature Composites Resins. , 2019, , .		1
81	Atomistic Simulations of Microelectronic Materials: Prediction of Mechanical, Thermal, and Electrical Properties. , 2012, , 3-24.		0
82	Fluorine coatings for nanoimprint lithography masks. , 2014, , .		0
83	Optical simulations for fractional fluorine terminated coatings on nanoimprint lithography masks. , 2015, , .		0
84	Generative machine learning for accelerated discovery of OLED materials. , 2021, , .		0
85	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