Alister J Page

List of Publications by Year in Descending Order

110 papers	3,189 citations	29 h-index	53 g-index
116 ext. papers	3,840 ext. citations	6.5 avg, IF	5.48 L-index

#	Paper	IF	Citations
110	First-Principles Thermochemical Properties of Hexagonal and Cubic Phase BaMnO3. *Materials Today Communications*, **2022**, 103453	2.5	0
109	Understanding specific ion effects and the Hofmeister series.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	13
108	Ion Specificity in the Measured Concentration Depth Profile of Ions at the Vapor-Glycerol Interface. *Journal of Colloid and Interface Science*, **2022**,	9.3	1
107	The electrostatic origins of specific ion effects: quantifying the Hofmeister series for anions.. *Chemical Science*, **2021**, 12, 15007-15015	9.4	9
106	Reaction pathways in the solid state and the Hubbard U correction. *Journal of Chemical Physics*, **2021**, 154, 124121	3.9	2
105	Cytotoxicity of Tin(IV)-based compounds: A review. *Polyhedron*, **2021**, 198, 115069	2.7	2
104	Group and Period-Based Representations for Improved Machine Learning Prediction of Heterogeneous Alloy Catalysts. *Journal of Physical Chemistry Letters*, **2021**, 12, 5156-5162	6.4	4
103	Low-Cost Pt Alloys for Heterogeneous Catalysis Predicted by Density Functional Theory and Active Learning. *Journal of Physical Chemistry Letters*, **2021**, 12, 7305-7311	6.4	1
102	Thermochemical stabilities of giant fullerenes using density functional tight binding theory and isodesmic-type reactions. *Journal of Computational Chemistry*, **2021**, 42, 222-230	3.5	4
101	Anion ordering and vacancy defects in niobium perovskite oxynitrides. *Materials Advances*, **2021**, 2, 2398-2407	3.4	
100	Initial competing chemical pathways during floating catalyst chemical vapor deposition carbon nanotube growth. *Journal of Applied Physics*, **2021**, 129, 044302	2.5	7
99	Energy and Charge Transfer at the Boron Nitride Nanotube–Catalyst Growth Interface. *Journal of Physical Chemistry C*, **2020**, 124, 11662-11668	3.8	1
98	Scalable growth of single-walled carbon nanotubes with a highly uniform structure. *Nanoscale*, **2020**, 12, 12263-12267	7.7	8
97	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *Journal of Chemical Physics*, **2020**, 152, 124101	3.9	210
96	Selective cytotoxicity of organotin(IV) compounds with 2,3-dihydroxybenzyldithiocarbazate Schiff bases. *Research on Chemical Intermediates*, **2020**, 46, 2351-2379	2.8	2
95	The Hubbard-U correction and optical properties of d metal oxide photocatalysts. *Journal of Chemical Physics*, **2020**, 153, 224116	3.9	5
94	Homoleptic tin(IV) compounds containing tridentate ONS dithiocarbazate Schiff bases: Synthesis, X-ray crystallography, DFT and cytotoxicity studies. *Journal of Molecular Structure*, **2020**, 1205, 127635	3.4	7

93	Hybrid Low-Dimensional Carbon Allotropes Formed in Gas Phase. *Advanced Functional Materials*, **2020**, 30, 2005016	15.6	5
92	Electronic Structure and High-Temperature Thermochemistry of Oxygen-Deficient BaMO3 (M = Ti Cu) Perovskites. *Journal of Physical Chemistry C*, **2020**, 124, 27055-27063	3.8	2
91	Tin(IV) compounds of tridentate thiosemicarbazone Schiff bases: Synthesis, characterization, in-silico analysis and in vitro cytotoxicity. *Polyhedron*, **2020**, 189, 114729	2.7	7
90	Experimental, computational and thermodynamic studies in perovskites metal oxides for thermochemical fuel production: A review. *International Journal of Hydrogen Energy*, **2020**, 45, 12653-12679	6.7	17
89	Defect Engineering for Photocatalysis: From Ternary to Perovskite Oxynitrides. *ChemNanoMat*, **2020**, 6, 708-719	3.5	9
88	Improved Representations of Heterogeneous Carbon Reforming Catalysis Using Machine Learning. *Journal of Chemical Theory and Computation*, **2019**, 15, 6882-6894	6.4	10
87	Electronic structure and high-temperature thermochemistry of BaZrO perovskite from first-principles calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 12468-12476	3.6	3
86	Lewis Strength Determines Specific-Ion Effects in Aqueous and Nonaqueous Solvents. *Journal of Physical Chemistry A*, **2019**, 123, 6420-6429	2.8	7
85	Catalyst- and Etchant-Dependent Mechanisms of Single-Walled Carbon Nanotube Nucleation during Chemical Vapor Deposition. *Journal of Physical Chemistry C*, **2019**, 123, 10622-10629	3.8	2
84	Vacancy diffusion barriers in TaON and Ta3N5 water-splitting photocatalysts. *Journal of Materials Chemistry A*, **2019**, 7, 13029-13035	13	15
83	New Phosphorene by Phase Combination with Tunable Electronic and Mechanical Properties. *Journal of Physical Chemistry C*, **2019**, 123, 10788-10794	3.8	9
82	Polymer solvation in choline chloride deep eutectic solvents modulated by the hydrogen bond donor. *Journal of Molecular Liquids*, **2019**, 279, 584-593	6	12
81	Boron Nitride Nanotube Nucleation via Network Fusion during Catalytic Chemical Vapor Deposition. *Journal of the American Chemical Society*, **2019**, 141, 13385-13393	16.4	12
80	Boron Nitride Nanotube Nucleation during Ni-Catalyzed Boron Oxide Chemical Vapor Deposition. *Journal of Physical Chemistry C*, **2019**, 123, 27875-27883	3.8	5
79	How does acetonitrile modulate single-walled carbon nanotube diameter during CVD growth?. *Carbon*, **2019**, 146, 535-541	10.4	7
78	-Vanillin Derived Schiff Bases and Their Organotin(IV) Compounds: Synthesis, Structural Characterisation, In-Silico Studies and Cytotoxicity. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	18
77	Effect of halides on the solvation of poly(ethylene oxide) in the ionic liquid propylammonium nitrate. *Journal of Colloid and Interface Science*, **2019**, 534, 649-654	9.3	5
76	Chiral-selective etching effects on carbon nanotube growth at edge carbon atoms. *Journal of Computational Chemistry*, **2019**, 40, 375-380	3.5	4

75	Performance of DFT for C Isomerization Energies: A Noticeable Exception to Jacob's Ladder. *Journal of Physical Chemistry A*, **2019**, 123, 257-266	2.8	13
74	Accurate Thermochemical and Kinetic Stabilities of C Isomers. *Journal of Physical Chemistry A*, **2018**, 122, 4768-4777	2.8	7
73	Nanostructure of propylammonium nitrate in the presence of poly(ethylene oxide) and halide salts. *Journal of Chemical Physics*, **2018**, 148, 193826	3.9	5
72	NO Solvation Structure in Choline Chloride Deep Eutectic Solvents-The Role of the Hydrogen Bond Donor. *Journal of Physical Chemistry B*, **2018**, 122, 4336-4344	3.4	22
71	Inducing regioselective chemical reactivity in graphene with alkali metal intercalation. *Physical Chemistry Chemical Physics*, **2018**, 20, 19987-19994	3.6	3
70	Synthesis, characterisation and structure determination of 3-[(1Z)-{2-[bis({[(2-methylphenyl)methyl]sulfanyl})methylidene]hydrazin-1-ylidene}methyl]benzene-1,2-diol. *Journal of Molecular Structure*, **2018**, 1171, 650-657	3.4	2
69	The influence of hydrogen on transition metal - Catalysed graphene nucleation. *Carbon*, **2018**, 128, 215-223	6.2	8
68	Density functional tight binding-based free energy simulations in the DFTB+ program. *Journal of Computational Chemistry*, **2018**, 39, 2452-2458	3.5	13
67	Boron Nitride Nucleation Mechanism during Chemical Vapor Deposition. *Journal of Physical Chemistry C*, **2018**, 122, 24341-24349	3.8	13
66	Oxygen Vacancy Defect Migration in Titanate Perovskite Surfaces: Effect of the A-Site Cations. *Journal of Physical Chemistry C*, **2018**, 122, 14590-14597	3.8	14
65	Effect of ammonia on chemical vapour deposition and carbon nanotube nucleation mechanisms. *Nanoscale*, **2017**, 9, 1727-1737	7.7	7
64	Nanostructure, hydrogen bonding and rheology in choline chloride deep eutectic solvents as a function of the hydrogen bond donor. *Physical Chemistry Chemical Physics*, **2017**, 19, 3297-3306	3.6	187
63	Catalytic CVD synthesis of boron nitride and carbon nanomaterials - synergies between experiment and theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 26466-26494	3.6	22
62	Chiral-Selective Carbon Nanotube Etching with Ammonia: A Quantum Chemical Investigation. *Journal of Physical Chemistry C*, **2016**, 120, 19862-19870	3.8	7
61	Spanning the Parameter Space of Chemical Vapor Deposition Graphene Growth with Quantum Chemical Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 13851-13864	3.8	12
60	Formation of persistent organic pollutants from 2,4,5-trichlorothiophenol combustion: a density functional theory investigation. *Journal of Molecular Modeling*, **2016**, 22, 128	2	6
59	General H2 Activation Modes for Lewis Acid Transition Metal Bifunctional Catalysts. *ACS Catalysis*, **2016**, 6, 1655-1662	13.1	64
58	Nanostructure of Deep Eutectic Solvents at Graphite Electrode Interfaces as a Function of Potential. *Journal of Physical Chemistry C*, **2016**, 120, 2225-2233	3.8	43

57	A global reaction route mapping-based kinetic Monte Carlo algorithm. *Journal of Chemical Physics*, **2016**, 145, 024105	3.9	11
56	The influence of magnetic moment on carbon nanotube nucleation. *Carbon*, **2016**, 105, 136-143	10.4	7
55	Theoretical analysis of structural diversity of covalent organic framework: Stacking isomer structures thermodynamics and kinetics. *Chemical Physics Letters*, **2016**, 664, 101-107	2.5	10
54	Quantum Chemical Simulation of Carbon Nanotube Nucleation on Al2O3 Catalysts via CH4 Chemical Vapor Deposition. *Journal of the American Chemical Society*, **2015**, 137, 9281-8	16.4	24
53	Formation of chlorobenzenes by oxidative thermal decomposition of 1,3-dichloropropene. *Combustion and Flame*, **2015**, 162, 2414-2421	5.3	11
52	Insights into carbon nanotube and graphene formation mechanisms from molecular simulations: a review. *Reports on Progress in Physics*, **2015**, 78, 036501	14.4	80
51	The ONIOM Method and Its Applications. *Chemical Reviews*, **2015**, 115, 5678-796	68.1	671
50	Quantum Chemical Molecular Dynamics Simulations of 1,3-Dichloropropene Combustion. *Journal of Physical Chemistry A*, **2015**, 119, 9307-16	2.8	10
49	Structure and absorption in C60⊇inc tetra-phenylporphyrin composite materials: A computational study. *Chemical Physics Letters*, **2015**, 620, 1-6	2.5	
48	Nearly exclusive growth of small diameter semiconducting single-wall carbon nanotubes from organic chemistry synthetic end-cap molecules. *Nano Letters*, **2015**, 15, 586-95	11.5	69
47	Nanostructure of [Li(G4)] TFSI and [Li(G4)] NO3 solvate ionic liquids at HOPG and Au(111) electrode interfaces as a function of potential. *Physical Chemistry Chemical Physics*, **2015**, 17, 325-33	3.6	53
46	Crystalline Ni3C as both carbon source and catalyst for graphene nucleation: a QM/MD study. *Scientific Reports*, **2015**, 5, 12091	4.9	30
45	Formation of benzofuran and chlorobenzofuran from 1,3-dichloropropene: A quantum chemical investigation. *International Journal of Quantum Chemistry*, **2015**, 115, 1739-1745	2.1	2
44	Combined friction force microscopy and quantum chemical investigation of the tribotronic response at the propylammonium nitrate-graphite interface. *Physical Chemistry Chemical Physics*, **2015**, 17, 16047-52	3.6	19
43	Graphene Nucleation from Amorphous Nickel Carbides: QM/MD Studies on the Role of Subsurface Carbon Density. *Journal of Physical Chemistry C*, **2014**, 118, 11078-11084	3.8	24
42	Step-edge self-assembly during graphene nucleation on a nickel surface: QM/MD simulations. *Nanoscale*, **2014**, 6, 140-4	7.7	22
41	3-Dimensional atomic scale structure of the ionic liquid-graphite interface elucidated by AM-AFM and quantum chemical simulations. *Nanoscale*, **2014**, 6, 8100-6	7.7	65
40	Assessment of the Density Functional Tight Binding Method for Protic Ionic Liquids. *Journal of Chemical Theory and Computation*, **2014**, 10, 4633-4643	6.4	36

39	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. *Chemical Science*, **2014**, 5, 3493-3500	9.4	36
38	Combined STM, AFM, and DFT Study of the Highly Ordered Pyrolytic Graphite/1-Octyl-3-methyl-imidazolium Bis(trifluoromethylsulfonyl)imide Interface. *Journal of Physical Chemistry C*, **2014**, 118, 10833-10843	3.8	59
37	Stochastic structure determination for conformationally flexible heterogenous molecular clusters: application to ionic liquids. *Journal of Computational Chemistry*, **2013**, 34, 2591-600	3.5	33
36	Temperature Dependence of Catalyst-Free Chirality-Controlled Single-Walled Carbon Nanotube Growth from Organic Templates. *Journal of Physical Chemistry Letters*, **2013**, 4, 3176-3180	6.4	10
35	Revealing the Dual Role of Hydrogen for Growth Inhibition and Defect Healing in Polycyclic Aromatic Hydrocarbon Formation: QM/MD Simulations. *Journal of Physical Chemistry Letters*, **2013**, 4, 2323-2327	6.4	15
34	Carbon Coating Precedes SWCNT Nucleation on Silicon Nanoparticles: Insights from QM/MD Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 4238-4244	3.8	11
33	Quantum chemical investigation of epoxide and ether groups in graphene oxide and their vibrational spectra. *Physical Chemistry Chemical Physics*, **2013**, 15, 3725-35	3.6	39
32	Nucleation of Graphene Precursors on Transition Metal Surfaces: Insights from Theoretical Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 14858-14864	3.8	38
31	Sub-surface nucleation of graphene precursors near a Ni(111) step-edge. *Chemical Communications*, **2012**, 48, 7937-9	5.8	37
30	Optimization of a Genetic Algorithm for the Functionalization of Fullerenes. *Journal of Chemical Theory and Computation*, **2012**, 8, 1841-51	6.4	13
29	Single-walled carbon nanotube growth from chiral carbon nanorings: prediction of chirality and diameter influence on growth rates. *Journal of the American Chemical Society*, **2012**, 134, 15887-96	16.4	48
28	Effects of Molecular Dynamics Thermostats on Descriptions of Chemical Nonequilibrium. *Journal of Chemical Theory and Computation*, **2012**, 8, 4019-28	6.4	11
27	Theoretical insights into chirality-controlled SWCNT growth from a cycloparaphenylene template. *ChemPhysChem*, **2012**, 13, 1479-85	3.2	26
26	Dynamics of local chirality during SWCNT growth: armchair versus zigzag nanotubes. *Journal of the American Chemical Society*, **2012**, 134, 9311-9	16.4	36
25	Atomistic Mechanism of Carbon Nanostructure Self-Assembly as Predicted by Nonequilibrium QM/MD Simulations **2012**, 103-172		4
24	Self-Consistent-Charge Density-Functional Tight-Binding/MD Simulation of Transition Metal Catalyst Particle Melting and Carbide Formation. *Journal of Computational and Theoretical Nanoscience*, **2011**, 8, 1755-1763	0.3	10
23	Thermal annealing of SiC nanoparticles induces SWNT nucleation: evidence for a catalyst-independent VSS mechanism. *Physical Chemistry Chemical Physics*, **2011**, 13, 15673-80	3.6	10
22	SWNT nucleation from carbon-coated SiO2 nanoparticles via a vapor-solid-solid mechanism. *Journal of the American Chemical Society*, **2011**, 133, 621-8	16.4	61

21	Template effect in the competition between Haeckelite and graphene growth on Ni(111): quantum chemical molecular dynamics simulations. *Journal of the American Chemical Society*, **2011**, 133, 18837-42	16.4	82
20	Do SiO2 and carbon-doped SiO2 nanoparticles melt? Insights from QM/MD simulations and ramifications regarding carbon nanotube growth. *Chemical Physics Letters*, **2011**, 508, 235-241	2.5	7
19	Polyyne Chain Growth and Ring Collapse Drives Ni-Catalyzed SWNT Growth: A QM/MD Investigation. *Journal of Physical Chemistry C*, **2010**, 114, 8206-8211	3.8	42
18	QM/MD simulation of SWNT nucleation on transition-metal carbide nanoparticles. *Journal of the American Chemical Society*, **2010**, 132, 15699-707	16.4	86
17	Mechanisms of single-walled carbon nanotube nucleation, growth, and healing determined using QM/MD methods. *Accounts of Chemical Research*, **2010**, 43, 1375-85	24.3	103
16	Trends in MH(2)(n+) ion-quadrupole complexes (M = Li, Be, Na, Mg, K, Ca; n = 1, 2) using ab initio methods. *Physical Chemistry Chemical Physics*, **2010**, 12, 13788-97	3.6	9
15	Comparison of single-walled carbon nanotube growth from Fe and Ni nanoparticles using quantum chemical molecular dynamics methods. *Carbon*, **2010**, 48, 3014-3026	10.4	40
14	Milestones in molecular dynamics simulations of single-walled carbon nanotube formation: A brief critical review. *Nano Research*, **2009**, 2, 755-767	10	45
13	Ab Initio rovibrational spectrum of the NaH2 + ion□quadrupole complex. *Theoretical Chemistry Accounts*, **2009**, 122, 87-100	1.9	10
12	Ab initio vibrational spectrum of (2□)He□MgH2+. *Chemical Physics Letters*, **2009**, 468, 299-306	2.5	1
11	Molecular dynamics simulation of the low-temperature partial oxidation of CH4. *Journal of Physical Chemistry A*, **2009**, 113, 1539-47	2.8	40
10	Defect Healing during Single-Walled Carbon Nanotube Growth: A Density-Functional Tight-Binding Molecular Dynamics Investigation. *Journal of Physical Chemistry C*, **2009**, 113, 20198-20207	3.8	57
9	Quantum chemical molecular dynamics simulation of single-walled carbon nanotube cap nucleation on an iron particle. *ACS Nano*, **2009**, 3, 3413-20	16.7	85
8	Ab initio study of ground state MH2, HMHe+ and MHe2(2+), M = Mg, Ca. *Physical Chemistry Chemical Physics*, **2008**, 10, 1285-91	3.6	10
7	Trends in low-lying electronic states of XH2 (X=Li, Na, K). *Computational and Theoretical Chemistry*, **2008**, 853, 53-57		3
6	Structural and energetic trends in Group-I and II hydrohelide cations. *Chemical Physics Letters*, **2008**, 465, 10-14	2.5	2
5	Ab initio electronic and rovibrational structure of MgH22+. *Chemical Physics*, **2008**, 351, 37-45	2.3	4
4	Rovibrational spectra of LiH2+, LiHD+ and LiD2+ determined from FCI property surfaces. *Journal of Physical Chemistry A*, **2007**, 111, 4478-88	2.8	21

3	Ab initio calculations of the electronic structure of the ground states of HBeHe+ and BeHe22+. *Chemical Physics Letters*, **2007**, 442, 194-200	2.5	6
2	Ab initio rovibrational spectra of , BeHD2+ and. *Molecular Physics*, **2007**, 105, 2527-2539	1.7	4
1	Ab initio properties and potential energy surface of the ground electronic state of . *Chemical Physics Letters*, **2006**, 429, 335-340	2.5	8