

# Alister J Page

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	The ONIOM Method and Its Applications. <i>Chemical Reviews</i> , <b>2015</b> , 115, 5678-796	68.1	671
109	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 124101	3.9	210
108	Nanostructure, hydrogen bonding and rheology in choline chloride deep eutectic solvents as a function of the hydrogen bond donor. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 3297-3306	3.6	187
107	Mechanisms of single-walled carbon nanotube nucleation, growth, and healing determined using QM/MD methods. <i>Accounts of Chemical Research</i> , <b>2010</b> , 43, 1375-85	24.3	103
106	QM/MD simulation of SWNT nucleation on transition-metal carbide nanoparticles. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 15699-707	16.4	86
105	Quantum chemical molecular dynamics simulation of single-walled carbon nanotube cap nucleation on an iron particle. <i>ACS Nano</i> , <b>2009</b> , 3, 3413-20	16.7	85
104	Template effect in the competition between Haeckelite and graphene growth on Ni(111): quantum chemical molecular dynamics simulations. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 18837-42	16.4	82
103	Insights into carbon nanotube and graphene formation mechanisms from molecular simulations: a review. <i>Reports on Progress in Physics</i> , <b>2015</b> , 78, 036501	14.4	80
102	Nearly exclusive growth of small diameter semiconducting single-wall carbon nanotubes from organic chemistry synthetic end-cap molecules. <i>Nano Letters</i> , <b>2015</b> , 15, 586-95	11.5	69
101	3-Dimensional atomic scale structure of the ionic liquid-graphite interface elucidated by AM-AFM and quantum chemical simulations. <i>Nanoscale</i> , <b>2014</b> , 6, 8100-6	7.7	65
100	General H <sub>2</sub> Activation Modes for Lewis Acid-Transition Metal Bifunctional Catalysts. <i>ACS Catalysis</i> , <b>2016</b> , 6, 1655-1662	13.1	64
99	SWNT nucleation from carbon-coated SiO <sub>2</sub> nanoparticles via a vapor-solid-solid mechanism. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 621-8	16.4	61
98	Combined STM, AFM, and DFT Study of the Highly Ordered Pyrolytic Graphite/1-Octyl-3-methyl-imidazolium Bis(trifluoromethylsulfonyl)imide Interface. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 10833-10843	3.8	59
97	Defect Healing during Single-Walled Carbon Nanotube Growth: A Density-Functional Tight-Binding Molecular Dynamics Investigation. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 20198-20207	3.8	57
96	Nanostructure of [Li(G4)] TFSI and [Li(G4)] NO <sub>3</sub> solvate ionic liquids at HOPG and Au(111) electrode interfaces as a function of potential. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 325-33	3.6	53
95	Single-walled carbon nanotube growth from chiral carbon nanorings: prediction of chirality and diameter influence on growth rates. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 15887-96	16.4	48
94	Milestones in molecular dynamics simulations of single-walled carbon nanotube formation: A brief critical review. <i>Nano Research</i> , <b>2009</b> , 2, 755-767	10	45

93	Nanostructure of Deep Eutectic Solvents at Graphite Electrode Interfaces as a Function of Potential. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 2225-2233	3.8	43
92	Polyne Chain Growth and Ring Collapse Drives Ni-Catalyzed SWNT Growth: A QM/MD Investigation. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 8206-8211	3.8	42
91	Molecular dynamics simulation of the low-temperature partial oxidation of CH <sub>4</sub> . <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 1539-47	2.8	40
90	Comparison of single-walled carbon nanotube growth from Fe and Ni nanoparticles using quantum chemical molecular dynamics methods. <i>Carbon</i> , <b>2010</b> , 48, 3014-3026	10.4	40
89	Quantum chemical investigation of epoxide and ether groups in graphene oxide and their vibrational spectra. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 3725-35	3.6	39
88	Nucleation of Graphene Precursors on Transition Metal Surfaces: Insights from Theoretical Simulations. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 14858-14864	3.8	38
87	Sub-surface nucleation of graphene precursors near a Ni(111) step-edge. <i>Chemical Communications</i> , <b>2012</b> , 48, 7937-9	5.8	37
86	Assessment of the Density Functional Tight Binding Method for Protic Ionic Liquids. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 4633-4643	6.4	36
85	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. <i>Chemical Science</i> , <b>2014</b> , 5, 3493-3500	9.4	36
84	Dynamics of local chirality during SWCNT growth: armchair versus zigzag nanotubes. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 9311-9	16.4	36
83	Stochastic structure determination for conformationally flexible heterogenous molecular clusters: application to ionic liquids. <i>Journal of Computational Chemistry</i> , <b>2013</b> , 34, 2591-600	3.5	33
82	Crystalline Ni <sub>3</sub> C as both carbon source and catalyst for graphene nucleation: a QM/MD study. <i>Scientific Reports</i> , <b>2015</b> , 5, 12091	4.9	30
81	Theoretical insights into chirality-controlled SWCNT growth from a cycloparaphenylene template. <i>ChemPhysChem</i> , <b>2012</b> , 13, 1479-85	3.2	26
80	Quantum Chemical Simulation of Carbon Nanotube Nucleation on Al <sub>2</sub> O <sub>3</sub> Catalysts via CH <sub>4</sub> Chemical Vapor Deposition. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 9281-8	16.4	24
79	Graphene Nucleation from Amorphous Nickel Carbides: QM/MD Studies on the Role of Subsurface Carbon Density. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 11078-11084	3.8	24
78	NO Solvation Structure in Choline Chloride Deep Eutectic Solvents-The Role of the Hydrogen Bond Donor. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 4336-4344	3.4	22
77	Step-edge self-assembly during graphene nucleation on a nickel surface: QM/MD simulations. <i>Nanoscale</i> , <b>2014</b> , 6, 140-4	7.7	22
76	Catalytic CVD synthesis of boron nitride and carbon nanomaterials - synergies between experiment and theory. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 26466-26494	3.6	22

75	Rovibrational spectra of LiH <sub>2</sub> <sup>+</sup> , LiHD <sup>+</sup> and LiD <sub>2</sub> <sup>+</sup> determined from FCI property surfaces. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 4478-88	2.8	21
74	Combined friction force microscopy and quantum chemical investigation of the tribotronic response at the propylammonium nitrate-graphite interface. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 16047-52	3.6	19
73	-Vanillin Derived Schiff Bases and Their Organotin(IV) Compounds: Synthesis, Structural Characterisation, In-Silico Studies and Cytotoxicity. <i>International Journal of Molecular Sciences</i> , <b>2019</b> , 20,	6.3	18
72	Experimental, computational and thermodynamic studies in perovskites metal oxides for thermochemical fuel production: A review. <i>International Journal of Hydrogen Energy</i> , <b>2020</b> , 45, 12653-12679	6.7	17
71	Vacancy diffusion barriers in TaON and Ta <sub>3</sub> N <sub>5</sub> water-splitting photocatalysts. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 13029-13035	13	15
70	Revealing the Dual Role of Hydrogen for Growth Inhibition and Defect Healing in Polycyclic Aromatic Hydrocarbon Formation: QM/MD Simulations. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 2323-2327	6.4	15
69	Oxygen Vacancy Defect Migration in Titanate Perovskite Surfaces: Effect of the A-Site Cations. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 14590-14597	3.8	14
68	Optimization of a Genetic Algorithm for the Functionalization of Fullerenes. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 1841-51	6.4	13
67	Performance of DFT for C Isomerization Energies: A Noticeable Exception to Jacob's Ladder. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 257-266	2.8	13
66	Density functional tight binding-based free energy simulations in the DFTB+ program. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 2452-2458	3.5	13
65	Boron Nitride Nucleation Mechanism during Chemical Vapor Deposition. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 24341-24349	3.8	13
64	Understanding specific ion effects and the Hofmeister series.. <i>Physical Chemistry Chemical Physics</i> , <b>2022</b> ,	3.6	13
63	Polymer solvation in choline chloride deep eutectic solvents modulated by the hydrogen bond donor. <i>Journal of Molecular Liquids</i> , <b>2019</b> , 279, 584-593	6	12
62	Spanning the Parameter Space of Chemical Vapor Deposition Graphene Growth with Quantum Chemical Simulations. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 13851-13864	3.8	12
61	Boron Nitride Nanotube Nucleation via Network Fusion during Catalytic Chemical Vapor Deposition. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 13385-13393	16.4	12
60	Formation of chlorobenzenes by oxidative thermal decomposition of 1,3-dichloropropene. <i>Combustion and Flame</i> , <b>2015</b> , 162, 2414-2421	5.3	11
59	Carbon Coating Precedes SWCNT Nucleation on Silicon Nanoparticles: Insights from QM/MD Simulations. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 4238-4244	3.8	11
58	Effects of Molecular Dynamics Thermostats on Descriptions of Chemical Nonequilibrium. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 4019-28	6.4	11

57	A global reaction route mapping-based kinetic Monte Carlo algorithm. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 024105	3.9	11
56	Improved Representations of Heterogeneous Carbon Reforming Catalysis Using Machine Learning. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 6882-6894	6.4	10
55	Quantum Chemical Molecular Dynamics Simulations of 1,3-Dichloropropene Combustion. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 9307-16	2.8	10
54	Temperature Dependence of Catalyst-Free Chirality-Controlled Single-Walled Carbon Nanotube Growth from Organic Templates. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 3176-3180	6.4	10
53	Self-Consistent-Charge Density-Functional Tight-Binding/MD Simulation of Transition Metal Catalyst Particle Melting and Carbide Formation. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2011</b> , 8, 1755-1763	0.3	10
52	Thermal annealing of SiC nanoparticles induces SWNT nucleation: evidence for a catalyst-independent VSS mechanism. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 15673-80	3.6	10
51	Ab Initio rovibrational spectrum of the NaH <sub>2</sub> + ion-quadrupole complex. <i>Theoretical Chemistry Accounts</i> , <b>2009</b> , 122, 87-100	1.9	10
50	Ab initio study of ground state MH <sub>2</sub> , HMHe <sup>+</sup> and MHe <sub>2</sub> (2 <sup>+</sup> ), M = Mg, Ca. <i>Physical Chemistry Chemical Physics</i> , <b>2008</b> , 10, 1285-91	3.6	10
49	Theoretical analysis of structural diversity of covalent organic framework: Stacking isomer structures thermodynamics and kinetics. <i>Chemical Physics Letters</i> , <b>2016</b> , 664, 101-107	2.5	10
48	New Phosphorene by Phase Combination with Tunable Electronic and Mechanical Properties. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 10788-10794	3.8	9
47	Trends in MH(2)(n <sup>+</sup> ) ion-quadrupole complexes (M = Li, Be, Na, Mg, K, Ca; n = 1, 2) using ab initio methods. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 13788-97	3.6	9
46	The electrostatic origins of specific ion effects: quantifying the Hofmeister series for anions.. <i>Chemical Science</i> , <b>2021</b> , 12, 15007-15015	9.4	9
45	Defect Engineering for Photocatalysis: From Ternary to Perovskite Oxynitrides. <i>ChemNanoMat</i> , <b>2020</b> , 6, 708-719	3.5	9
44	Scalable growth of single-walled carbon nanotubes with a highly uniform structure. <i>Nanoscale</i> , <b>2020</b> , 12, 12263-12267	7.7	8
43	Ab initio properties and potential energy surface of the ground electronic state of . <i>Chemical Physics Letters</i> , <b>2006</b> , 429, 335-340	2.5	8
42	The influence of hydrogen on transition metal - Catalysed graphene nucleation. <i>Carbon</i> , <b>2018</b> , 128, 215-224	2.4	8
41	Effect of ammonia on chemical vapour deposition and carbon nanotube nucleation mechanisms. <i>Nanoscale</i> , <b>2017</b> , 9, 1727-1737	7.7	7
40	Lewis Strength Determines Specific-Ion Effects in Aqueous and Nonaqueous Solvents. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 6420-6429	2.8	7

39	Accurate Thermochemical and Kinetic Stabilities of C Isomers. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 4768-4777	2.8	7
38	Chiral-Selective Carbon Nanotube Etching with Ammonia: A Quantum Chemical Investigation. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 19862-19870	3.8	7
37	Do SiO <sub>2</sub> and carbon-doped SiO <sub>2</sub> nanoparticles melt? Insights from QM/MD simulations and ramifications regarding carbon nanotube growth. <i>Chemical Physics Letters</i> , <b>2011</b> , 508, 235-241	2.5	7
36	Homoleptic tin(IV) compounds containing tridentate ONS dithiocarbazate Schiff bases: Synthesis, X-ray crystallography, DFT and cytotoxicity studies. <i>Journal of Molecular Structure</i> , <b>2020</b> , 1205, 127635	3.4	7
35	Tin(IV) compounds of tridentate thiosemicarbazone Schiff bases: Synthesis, characterization, in-silico analysis and in vitro cytotoxicity. <i>Polyhedron</i> , <b>2020</b> , 189, 114729	2.7	7
34	The influence of magnetic moment on carbon nanotube nucleation. <i>Carbon</i> , <b>2016</b> , 105, 136-143	10.4	7
33	How does acetonitrile modulate single-walled carbon nanotube diameter during CVD growth?. <i>Carbon</i> , <b>2019</b> , 146, 535-541	10.4	7
32	Initial competing chemical pathways during floating catalyst chemical vapor deposition carbon nanotube growth. <i>Journal of Applied Physics</i> , <b>2021</b> , 129, 044302	2.5	7
31	Formation of persistent organic pollutants from 2,4,5-trichlorothiophenol combustion: a density functional theory investigation. <i>Journal of Molecular Modeling</i> , <b>2016</b> , 22, 128	2	6
30	Ab initio calculations of the electronic structure of the ground states of HBeHe <sup>+</sup> and BeHe <sub>2</sub> <sup>2+</sup> . <i>Chemical Physics Letters</i> , <b>2007</b> , 442, 194-200	2.5	6
29	Nanostructure of propylammonium nitrate in the presence of poly(ethylene oxide) and halide salts. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 193826	3.9	5
28	Boron Nitride Nanotube Nucleation during Ni-Catalyzed Boron Oxide Chemical Vapor Deposition. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 27875-27883	3.8	5
27	The Hubbard-U correction and optical properties of d metal oxide photocatalysts. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 224116	3.9	5
26	Hybrid Low-Dimensional Carbon Allotropes Formed in Gas Phase. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 2005016	15.6	5
25	Effect of halides on the solvation of poly(ethylene oxide) in the ionic liquid propylammonium nitrate. <i>Journal of Colloid and Interface Science</i> , <b>2019</b> , 534, 649-654	9.3	5
24	Atomistic Mechanism of Carbon Nanostructure Self-Assembly as Predicted by Nonequilibrium QM/MD Simulations <b>2012</b> , 103-172		4
23	Ab initio electronic and rovibrational structure of MgH <sub>2</sub> <sup>2+</sup> . <i>Chemical Physics</i> , <b>2008</b> , 351, 37-45	2.3	4
22	Ab initio rovibrational spectra of , BeHD <sub>2</sub> <sup>+</sup> and. <i>Molecular Physics</i> , <b>2007</b> , 105, 2527-2539	1.7	4

21	Group and Period-Based Representations for Improved Machine Learning Prediction of Heterogeneous Alloy Catalysts. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 5156-5162	6.4	4
20	Chiral-selective etching effects on carbon nanotube growth at edge carbon atoms. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 375-380	3.5	4
19	Thermochemical stabilities of giant fullerenes using density functional tight binding theory and isodesmic-type reactions. <i>Journal of Computational Chemistry</i> , <b>2021</b> , 42, 222-230	3.5	4
18	Electronic structure and high-temperature thermochemistry of BaZrO perovskite from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 12468-12476	3.6	3
17	Inducing regioselective chemical reactivity in graphene with alkali metal intercalation. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 19987-19994	3.6	3
16	Trends in low-lying electronic states of XH <sub>2</sub> (X=Li, Na, K). <i>Computational and Theoretical Chemistry</i> , <b>2008</b> , 853, 53-57		3
15	Catalyst- and Etchant-Dependent Mechanisms of Single-Walled Carbon Nanotube Nucleation during Chemical Vapor Deposition. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 10622-10629	3.8	2
14	Selective cytotoxicity of organotin(IV) compounds with 2,3-dihydroxybenzylidithiocarbamate Schiff bases. <i>Research on Chemical Intermediates</i> , <b>2020</b> , 46, 2351-2379	2.8	2
13	Synthesis, characterisation and structure determination of 3-[(1Z)-{2-[bis({[(2-methylphenyl)methyl]sulfanyl})methylidene]hydrazin-1-ylidene)methyl]benzene-1,2-diol. <i>Journal of Molecular Structure</i> , <b>2018</b> , 1171, 650-657	3.4	2
12	Formation of benzofuran and chlorobenzofuran from 1,3-dichloropropene: A quantum chemical investigation. <i>International Journal of Quantum Chemistry</i> , <b>2015</b> , 115, 1739-1745	2.1	2
11	Structural and energetic trends in Group-I and II hydrohelide cations. <i>Chemical Physics Letters</i> , <b>2008</b> , 465, 10-14	2.5	2
10	Electronic Structure and High-Temperature Thermochemistry of Oxygen-Deficient BaMO <sub>3</sub> (M = Ti □ Cu) Perovskites. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 27055-27063	3.8	2
9	Reaction pathways in the solid state and the Hubbard U correction. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 124121	3.9	2
8	Cytotoxicity of Tin(IV)-based compounds: A review. <i>Polyhedron</i> , <b>2021</b> , 198, 115069	2.7	2
7	Energy and Charge Transfer at the Boron Nitride Nanotube Catalyst Growth Interface. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 11662-11668	3.8	1
6	Ab initio vibrational spectrum of (2 $\pi$ )HeMgH <sub>2</sub> <sup>+</sup> . <i>Chemical Physics Letters</i> , <b>2009</b> , 468, 299-306	2.5	1
5	Low-Cost Pt Alloys for Heterogeneous Catalysis Predicted by Density Functional Theory and Active Learning. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 7305-7311	6.4	1
4	Ion Specificity in the Measured Concentration Depth Profile of Ions at the Vapor-Glycerol Interface. <i>Journal of Colloid and Interface Science</i> , <b>2022</b> ,	9.3	1



- 3 First-Principles Thermochemical Properties of Hexagonal and Cubic Phase BaMnO<sub>3</sub>. *Materials Today Communications*, **2022**, 103453 2.5 0
- 2 Structure and absorption in C<sub>60</sub>/zinc tetra-phenylporphyrin composite materials: A computational study. *Chemical Physics Letters*, **2015**, 620, 1-6 2.5
- 1 Anion ordering and vacancy defects in niobium perovskite oxynitrides. *Materials Advances*, **2021**, 2, 2398-2407 3.5