Michael J. Ford

List of Publications by Year in Descending Order

141 papers	5,170 citations	37 h-index	68 g-index
152 ext. papers	6,053 ext. citations	5.9 avg, IF	5.96 L-index

#	Paper	IF	Citations
141	Density functionals with asymptotic-potential corrections are required for the simulation of spectroscopic properties of materials.. *Chemical Science*, **2022**, 13, 1492-1503	9.4	0
140	A bright future for engineering piezoelectric 2D crystals.. *Chemical Society Reviews*, **2021**,	58.5	3
139	Accurate prediction of the properties of materials using the CAM-B3LYP density functional. *Journal of Computational Chemistry*, **2021**, 42, 1486-1497	3.5	11
138	Identifying carbon as the source of visible single-photon emission from hexagonal boron nitride. *Nature Materials*, **2021**, 20, 321-328	27	78
137	Modeling of metal nanoparticles: Development of neural-network interatomic potential inspired by features of the modified embedded-atom method. *Physical Review B*, **2020**, 102,	3.3	1
136	Role of knock-on in electron beam induced etching of diamond. *Carbon*, **2020**, 164, 51-58	10.4	2
135	Single-photon emitters in hexagonal boron nitride: a review of progress. *Reports on Progress in Physics*, **2020**, 83, 044501	14.4	52
134	Photoluminescence, photophysics, and photochemistry of the VB□ defect in hexagonal boron nitride. *Physical Review B*, **2020**, 102,	3.3	21
133	Theoretical spectroscopy of the VNNB defect in hexagonal boron nitride. *Physical Review B*, **2020**, 102,	3.3	8
132	Observation of near-infrared sub-Poissonian photon emission in hexagonal boron nitride at room temperature. *APL Photonics*, **2020**, 5, 076103	5.2	7
131	Convergence of Defect Energetics Calculations. *Journal of Physical Chemistry C*, **2020**, 124, 21178-21183	3.8	9
130	Edge effects on optically detected magnetic resonance of vacancy defects in hexagonal boron nitride. *Communications Physics*, **2020**, 3,	5.4	13
129	High Throughput Screening of Millions of van der Waals Heterostructures for Superlubricant Applications. *Advanced Theory and Simulations*, **2020**, 3, 2000029	3.5	4
128	Efficient Production of Phosphorene Nanosheets via Shear Stress Mediated Exfoliation for Low-Temperature Perovskite Solar Cells. *Small Methods*, **2019**, 3, 1800521	12.8	42
127	Structure, stability and water adsorption on ultra-thin TiO supported on TiN. *Physical Chemistry Chemical Physics*, **2019**, 21, 25344-25361	3.6	2
126	Efficient Prediction of Structural and Electronic Properties of Hybrid 2D Materials Using Complementary DFT and Machine Learning Approaches. *Advanced Theory and Simulations*, **2019**, 2, 1800128	3.5	34
125	Anisotropic functionalization of upconversion nanoparticles. *Chemical Science*, **2018**, 9, 4352-4358	9.4	31

124	Defect states in hexagonal boron nitride: Assignments of observed properties and prediction of properties relevant to quantum computation. *Physical Review B*, **2018**, 97,	3.3	81
123	Electrocatalytic Activity of a 2D Phosphorene-Based Heteroelectrocatalyst for Photoelectrochemical Cells. *Angewandte Chemie - International Edition*, **2018**, 57, 2644-2647	16.4	39
122	Electrocatalytic Activity of a 2D Phosphorene-Based Heteroelectrocatalyst for Photoelectrochemical Cells. *Angewandte Chemie*, **2018**, 130, 2674-2677	3.6	8
121	Understanding and Calibrating Density-Functional-Theory Calculations Describing the Energy and Spectroscopy of Defect Sites in Hexagonal Boron Nitride. *Journal of Chemical Theory and Computation*, **2018**, 14, 1602-1613	6.4	42
120	Magnetic properties of stoichiometric and defective CoS. *Physical Chemistry Chemical Physics*, **2018**, 20, 2356-2362	3.6	11
119	Single photon emission from plasma treated 2D hexagonal boron nitride. *Nanoscale*, **2018**, 10, 7957-7965	7.7	64
118	Evaluation of van der Waals density functionals for layered materials. *Physical Review Materials*, **2018**, 2,	3.2	47
117	Ab Initio Investigation of Water Adsorption and Hydrogen Evolution on CoS and CoS Low-Index Surfaces. *ACS Omega*, **2018**, 3, 12215-12228	3.9	11
116	van der Waals forces control ferroelectric-antiferroelectric ordering in CuInPS and CuBiPSe laminar materials. *Chemical Science*, **2018**, 9, 7620-7627	9.4	21
115	van der Waals Forces Control the Internal Chemical Structure of Monolayers within the Lamellar Materials CuInP2S6 and CuBiP2Se6. *Journal of Physical Chemistry C*, **2018**, 122, 22675-22687	3.8	11
114	High-performance Na ion cathodes based on the ubiquitous and reversible O redox reaction. *Journal of Materials Chemistry A*, **2018**, 6, 24120-24127	13	5
113	Superconductivity in intercalated buckled two-dimensional materials: KGe. *Physical Chemistry Chemical Physics*, **2018**, 20, 24027-24032	3.6	1
112	Indirect excitons in hydrogen-doped ZnO. *Journal Physics D: Applied Physics*, **2017**, 50, 115104	3	2
111	Robust Solid-State Quantum System Operating at 800 K. *ACS Photonics*, **2017**, 4, 768-773	6.3	68
110	Competition of van der Waals and chemical forces on gold–sulfur surfaces and nanoparticles. *Nature Reviews Chemistry*, **2017**, 1,	34.6	72
109	Sulfur ligand mediated electrochemistry of gold surfaces and nanoparticles: What, how, and why. *Current Opinion in Electrochemistry*, **2017**, 1, 7-15	7.2	26
108	Efficiency Enhancement of Single-Walled Carbon Nanotube-Silicon Heterojunction Solar Cells Using Microwave-Exfoliated Few-Layer Black Phosphorus. *Advanced Functional Materials*, **2017**, 27, 1704488	15.6	36
107	Tunable and high-purity room temperature single-photon emission from atomic defects in hexagonal boron nitride. *Nature Communications*, **2017**, 8, 705	17.4	226

106	First-principles investigation of quantum emission from hBN defects. *Nanoscale*, **2017**, 9, 13575-13582	7.7	122
105	Layer-by-Layer Assembly of Multilayer Thin Films for Organic Optoelectronic Devices. *Small Methods*, **2017**, 1, 1700264	12.8	29
104	Efficient and Fast Synthesis of Few-Layer Black Phosphorus via Microwave-Assisted Liquid-Phase Exfoliation. *Small Methods*, **2017**, 1, 1700260	12.8	47
103	Surface Adsorption **2017**, 387-416		3
102	Robust Multicolor Single Photon Emission from Point Defects in Hexagonal Boron Nitride. *ACS Nano*, **2016**, 10, 7331-8	16.7	285
101	Problems, successes and challenges for the application of dispersion-corrected density-functional theory combined with dispersion-based implicit solvent models to large-scale hydrophobic self-assembly and polymorphism. *Molecular Simulation*, **2016**, 42, 494-510	2	13
100	From Chaos to Order: Chain-Length Dependence of the Free Energy of Formation of Meso-tetraalkylporphyrin Self-Assembled Monolayer Polymorphs. *Journal of Physical Chemistry C*, **2016**, 120, 1739-1748	3.8	13
99	Quantum emission from hexagonal boron nitride monolayers. *Nature Nanotechnology*, **2016**, 11, 37-41	28.7	675
98	Quantum Emission from Hexagonal Boron Nitride Monolayers **2016**,		1
97	Ultra-bright emission from hexagonal boron nitride defects as a new platform for bio-imaging and bio-labelling **2016**,		1
96	Gold surfaces and nanoparticles are protected by Au(0)-thiyl species and are destroyed when Au(I)-thiolates form. *Proceedings of the National Academy of Sciences of the United States of America* , **2016**, 113, E1424-33	11.5	83
95	Localized Probing of Gas Molecule Adsorption Energies and Desorption Attempt Frequencies. *Journal of Physical Chemistry C*, **2015**, 119, 15948-15953	3.8	11
94	A priori calculations of the free energy of formation from solution of polymorphic self-assembled monolayers. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E6101-10	11.5	32
93	Electron-Beam-Induced Deposition as a Technique for Analysis of Precursor Molecule Diffusion Barriers and Prefactors. *ACS Applied Materials & Interfaces*, **2015**, 7, 21408-15	9.5	5
92	Phase transitions and optical properties of the semiconducting and metallic phases of single-layer MoS *Nanotechnology*, **2015**, 26, 435705	3.4	12
91	Determination of the elastic properties of graphene by indentation and the validity of classical models of indentation. *Journal of Physics Condensed Matter*, **2014**, 26, 015307	1.8	8
90	Local plasmon resonances of metal-in-metal core-shells. *Optics Express*, **2014**, 22, 3186-98	3.3	14
89	Phonon pressure coefficients and deformation potentials of wurtzite AlN determined by uniaxial pressure-dependent Raman measurements. *Physical Review B*, **2014**, 90,	3.3	13

88	Li-ion adsorption and diffusion on two-dimensional silicon with defects: a first principles study. *ACS Applied Materials & Interfaces*, **2013**, 5, 10690-5	9.5	63
87	Hydrogen adsorption capacity of adatoms on double carbon vacancies of graphene: A trend study from first principles. *Physical Review B*, **2013**, 87,	3.3	85
86	Molecular rectifiers based on donor/acceptor assemblies: effect of orientation of the components' magnetic moments. *Nanoscale*, **2013**, 5, 6518-24	7.7	6
85	Damping of Plasmons of Closely Coupled Sphere Chains Due to Disordered Gaps. *Journal of Physical Chemistry C*, **2012**, 116, 1335-1343	3.8	5
84	Mesoporous NiO crystals with dominantly exposed {110} reactive facets for ultrafast lithium storage. *Scientific Reports*, **2012**, 2, 924	4.9	138
83	Role of activated chemisorption in gas-mediated electron beam induced deposition. *Physical Review Letters*, **2012**, 109, 146103	7.4	31
82	Systematic study of bimodal suspensions of latex nanoparticles using dynamic light scattering. *Advanced Powder Technology*, **2011**, 22, 290-293	4.6	18
81	SIESTA: Properties and Applications **2011**, 367-395		1
80	A review of the optical properties of alloys and intermetallics for plasmonics. *Journal of Physics Condensed Matter*, **2010**, 22, 143201	1.8	195
79	Transmitting hertzian optical nanoantenna with free-electron feed. *Nano Letters*, **2010**, 10, 3250-2	11.5	36
78	Universal scaling of local plasmons in chains of metal spheres. *Optics Express*, **2010**, 18, 7528-42	3.3	26
77	Chemical analysis of the superatom model for sulfur-stabilized gold nanoparticles. *Journal of the American Chemical Society*, **2010**, 132, 8378-84	16.4	80
76	Designing materials for plasmonic systems: the alkali-noble intermetallics. *Journal of Physics Condensed Matter*, **2010**, 22, 095501	1.8	35
75	Plasmonic Resonances of Closely Coupled Gold Nanosphere Chains. *Journal of Physical Chemistry C*, **2009**, 113, 2784-2791	3.8	75
74	Rapid and Controllable Sintering of Gold Nanoparticle Inks at Room Temperature Using a Chemical Agent. *Journal of Physical Chemistry C*, **2009**, 113, 1325-1328	3.8	58
73	Optical properties of intermetallic compounds from first principles calculations: a search for the ideal plasmonic material. *Journal of Physics Condensed Matter*, **2009**, 21, 144211	1.8	40
72	Search for the Ideal Plasmonic Nanoshell: The Effects of Surface Scattering and Alternatives to Gold and Silver. *Journal of Physical Chemistry C*, **2009**, 113, 3041-3045	3.8	167
71	The effect of stretching thiyl□and ethynyl□Au molecular junctions. *Journal of Physics Condensed Matter*, **2008**, 20, 025207	1.8	13

70	Rectification in donor-acceptor molecular junctions. *Journal of Physics Condensed Matter*, **2008**, 20, 374106	1.8	22
69	First principles calculations using density matrix divide-and-conquer within the SIESTA methodology. *Journal of Physics Condensed Matter*, **2008**, 20, 294208	1.8	11
68	Tunable infrared absorption by metal nanoparticles: The case for gold rods and shells **2008**, 41, 5-14		53
67	Compton scattering study of electron momentum distribution in lithium fluoride using 662 keV gamma radiations. *Physica B: Condensed Matter*, **2008**, 403, 4309-4313	2.8	3
66	Ab initio molecular dynamical investigation of the finite temperature behavior of the tetrahedral Au19 and Au20 clusters. *Journal of Physical Chemistry A*, **2007**, 111, 10769-75	2.8	33
65	Ethynylbenzene monolayers on gold: a metal-molecule binding motif derived from a hydrocarbon. *Journal of the American Chemical Society*, **2007**, 129, 3533-8	16.4	29
64	Exploring the performance of molecular rectifiers: limitations and factors affecting molecular rectification. *Nano Letters*, **2007**, 7, 3018-22	11.5	30
63	Laser-induced assembly of gold nanoparticles into colloidal crystals. *Nanotechnology*, **2007**, 18, 365301	3.4	10
62	A plasmon-induced current loop in gold semi-shells. *Nanotechnology*, **2007**, 18, 235704	3.4	79
61	Active control of the optical properties of nanoscale coatings using 'smart' nanoparticles **2007**,		2
60	Plasmon absorption in nanospheres: A comparison of sodium, potassium, aluminium, silver and gold. *Physica B: Condensed Matter*, **2007**, 394, 184-187	2.8	92
59	Plasmonic heating and its possible exploitation in nanolithography. *Physica B: Condensed Matter*, **2007**, 394, 188-192	2.8	21
58	Electron tunneling in the presence of adsorbed molecules. *Surface Science*, **2007**, 601, 5715-5720	1.8	1
57	Stability of the tetrahedral motif for small gold clusters in the size range 16–24 atoms. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2007**, 140, 177-181	3.1	3
56	Ab initioand empirical studies on the asymmetry of molecular current–voltage characteristics. *Journal of Physics Condensed Matter*, **2007**, 19, 215206	1.8	11
55	The effect of reciprocal-space sampling and basis set quality on the calculated conductance of a molecular junction. *Molecular Simulation*, **2007**, 33, 897-904	2	7
54	Core-shell nanoparticles with self-regulating plasmonic functionality. *Physical Review B*, **2007**, 75,	3.3	28
53	Adsorption of Amine Compounds on the Au(111) Surface: A Density Functional Study. *Journal of Physical Chemistry C*, **2007**, 111, 13886-13891	3.8	115

52	Anisotropic Optical Properties of Semitransparent Coatings of Gold Nanocaps. *Advanced Functional Materials*, **2006**, 16, 1457-1461	15.6	40
51	A new class of self-assembled monolayers on gold using an alkynyl group as a linker **2006**,		1
50	**2006**,		1
49	Effect of dipole moment on current-voltage characteristics of single molecules **2006**,		1
48	Adsorption and dimerisation of thiol molecules on Au(111) using a Z-matrix approach in density functional theory. *Molecular Simulation*, **2006**, 32, 1219-1225	2	19
47	Adsorption of Benzene on Copper, Silver, and Gold Surfaces. *Journal of Chemical Theory and Computation*, **2006**, 2, 1093-105	6.4	130
46	Effect of composition and packing configuration on the dichroic optical properties of coinage metal nanorods. *Physical Chemistry Chemical Physics*, **2006**, 8, 3520-7	3.6	37
45	Implementation of a Z-matrix approach within the SIESTA periodic boundary conditions code and its application to surface adsorption. *Molecular Simulation*, **2006**, 32, 595-600	2	9
44	Optimization of plasmonic heating by gold nanospheres and nanoshells. *Journal of Physical Chemistry B*, **2006**, 110, 10701-7	3.4	127
43	THE APPLICATION OF GOLD SURFACES AND PARTICLES IN NANOTECHNOLOGY. *Surface Review and Letters*, **2006**, 13, 297-307	1.1	28
42	Controlled Assembly of 1,4-Phenylenedimethanethiol Molecular Nanostructures. *Chemistry of Materials*, **2006**, 18, 2376-2380	9.6	13
41	Melting in small gold clusters: a density functional molecular dynamics study. *Journal of Physics Condensed Matter*, **2006**, 18, 55-74	1.8	35
40	Measuring the electronic structure of disordered overlayers by electron momentum spectroscopy: the Cu/Si interface. *Surface and Interface Analysis*, **2006**, 38, 1236-1241	1.5	3
39	Prediction of increased tunneling current by bond length stretch in molecular break junctions. *Chemical Physics Letters*, **2006**, 429, 503-506	2.5	13
38	Theoretical study of ethynylbenzene adsorption on Au(111) and implications for a new class of self-assembled monolayer. *Journal of Physical Chemistry B*, **2005**, 109, 20387-92	3.4	58
37	Conduction, storage, and leakage in particle-on-SAM nanocapacitors. *IEEE Nanotechnology Magazine*, **2005**, 4, 406-414	2.6	9
36	Investigation of the optical properties of hollow aluminium nano-caps *Nanotechnology*, **2005**, 16, 3023-3028	3.4	30
35	Compton profile of polycrystalline sodium chloride and sodium fluoride. *Nuclear Instruments & Methods in Physics Research B*, **2005**, 234, 185-193	1.2	3

34	Growth Kinetics and Modeling of ZnO Nanoparticles. *Journal of Chemical Education*, **2005**, 82, 775	2.4	51
33	The effect of surface symmetry on the adsorption energetics of SCH3 on gold surfaces studied using Density Functional Theory. *Surface Science*, **2005**, 580, 19-29	1.8	35
32	Absorption energetics and simulation of STM images for fluorobenzene on the Cu(110) surface. *Modelling and Simulation in Materials Science and Engineering*, **2004**, 12, 1109-1120	2	2
31	Teaching Undergraduates Nanotechnology. *Materials Research Society Symposia Proceedings*, **2004**, 827, 151		1
30	Ab initio study of benzene adsorption on the Cu(110) surface and simulation of STM images. *Surface Science*, **2004**, 548, 29-40	1.8	39
29	Electronic band structure of calcium oxide. *Journal of Electron Spectroscopy and Related Phenomena* , **2004**, 141, 27-38	1.7	24
28	Low energy structures of gold nanoclusters in the size range 3□8 atoms. *Computational and Theoretical Chemistry*, **2004**, 686, 193-205		57
27	Design of nanocapacitors and associated materials challenges. *Current Applied Physics*, **2004**, 4, 250-254	2.6	6
26	Energy-efficient coatings in the NanohouseTM Initiative. *Current Applied Physics*, **2004**, 4, 381-384	2.6	1
25	Liquid-Crystal Displays: Fabrication and Measurement of a Twisted Nematic Liquid-Crystal Cell. *Journal of Chemical Education*, **2004**, 81, 854	2.4	13
24	Trends in the band structures of the group-I and -II oxides. *Journal of Chemical Physics*, **2004**, 120, 10799-806	3.9	16
23	Electronic band structure of beryllium oxide. *Journal of Physics Condensed Matter*, **2003**, 15, 3567-3581	1.8	42
22	Electron momentum spectroscopy and linear combination of atomic orbitals calculation of bulk Na2O. *Journal of Physics Condensed Matter*, **2003**, 15, 2155-2168	1.8	13
21	The electronic structure of Be and BeO: benchmark EMS measurements and LCAO calculations. *Journal of Physics and Chemistry of Solids*, **2003**, 64, 495-505	3.9	18
20	Energy and momentum resolved band structure of K2O : electron momentum spectroscopy and linear combination of atomic orbitals calculation. *Journal of Physics Condensed Matter*, **2003**, 15, 6955-6968	1.8	9
19	The electronic band structure of Li2O: testing theoretical predictions using electron momentum spectroscopy. *Journal of Physics Condensed Matter*, **2002**, 14, 3587-3598	1.8	23
18	Conduction band electronic structure of metallic beryllium. *Journal of Physics Condensed Matter*, **2001**, 13, 4203-4219	1.8	8
17	Time-resolved study of beryllium surface reactions using electron momentum spectroscopy of the core-level. *Surface Science*, **2001**, 495, 35-43	1.8	2

16	Preparation of a 10 nm thick single-crystal silicon membrane self-supporting over a diameter of 1 mm. *Applied Surface Science*, **2000**, 162-163, 359-367	6.7	11
15	The valence band structures of BeO, MgO, and CaO. *Journal of Chemical Physics*, **2000**, 113, 8175-8182	3.9	23
14	Energy-resolved momentum densities for the valence band of a nanoscale Si single crystal. *Journal of Physics Condensed Matter*, **2000**, 12, 125-136	1.8	16
13	Electronic band structure of metallic calcium measured by electron momentum spectroscopy. *Journal of Physics Condensed Matter*, **2000**, 12, 9407-9423	1.8	6
12	Electronic band structure of magnesium and magnesium oxide: experiment and theory. *Journal of Physics Condensed Matter*, **1999**, 11, 7507-7522	1.8	23
11	Electron-impact double ionization of magnesium. *Physical Review A*, **1998**, 57, 325-330	2.6	9
10	Valence-band energy-momentum densities of amorphous SiO2 by (e,2e) spectroscopy. *Physical Review B*, **1998**, 57, 4349-4357	3.3	12
9	Partitioning of Momentum in Electron-Impact Double Ionization **1997**, 85-92		
8	Partitioning of Momentum in Electron-Impact Double Ionization of Magnesium. *Physical Review Letters*, **1996**, 77, 2650-2653	7.4	11
7	(e,3e) observation of the angular correlation between ejected and Auger electrons in the double ionization of magnesium. *Physical Review A*, **1995**, 51, 418-423	2.6	17
6	Multiple detector triple coincidence spectrometer for (e,3e) electron impact double-ionization measurements. *Review of Scientific Instruments*, **1995**, 66, 3137-3143	1.7	22
5	Histogramming data acquisition system for an (e,2e) coincidence experiment. *Review of Scientific Instruments*, **1992**, 63, 1922-1926	1.7	9
4	The ejected-electron spectra of manganese and samarium vapour atoms arising from autoionizing and Auger transitions following electron impact excitation. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1990**, 23, 4247-4262	1.3	4
3	. *Journal of Physics B: Atomic and Molecular Physics*, **1987**, 20, 4241-4253		3
2	Quantum electrical characteristics of nanocapacitors		3
1	Active Learning in Bayesian Neural Networks for Bandgap Predictions of Novel Van der Waals Heterostructures. *Advanced Intelligent Systems*,2100080	6	1