

Benjamin J Morgan

List of Publications by Year in Descending Order

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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.

85
papers

4,321
citations

33
h-index

65
g-index

102
ext. papers

4,837
ext. citations

6.1
avg, IF

6.04
L-index

#	Paper	IF	Citations
85	Understanding fast-ion conduction in solid electrolytes. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2021 , 379, 20190451	3	2
84	Mechanistic Origin of Superionic Lithium Diffusion in Anion-Disordered LiPS Argyrodites. <i>Chemistry of Materials</i> , 2021 , 33, 2004-2018	9.6	21
83	Impact of Solution Chemistry on Growth and Structural Features of Mo-Substituted Spinel Iron Oxides. <i>Inorganic Chemistry</i> , 2021 , 60, 7217-7227	5.1	2
82	Overscreening and Underscreening in Solid-Electrolyte Grain Boundary Space-Charge Layers. <i>Physical Review Letters</i> , 2021 , 127, 135502	7.4	1
81	Evidence for a Solid-Electrolyte Inductive Effect in the Superionic Conductor LiGeSnPS. <i>Journal of the American Chemical Society</i> , 2020 , 142, 21210-21219	16.4	23
80	Atomic Insights into Aluminium-Ion Insertion in Defective Anatase for Batteries. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 19247-19253	16.4	13
79	Atomic Insights into Aluminium-Ion Insertion in Defective Anatase for Batteries. <i>Angewandte Chemie</i> , 2020 , 132, 19409-19415	3.6	0
78	Low-cost descriptors of electrostatic and electronic contributions to anion redox activity in batteries. <i>IOP SciNotes</i> , 2020 , 1, 024805	1.2	3
77	Native Defects and Their Doping Response in the Lithium Solid Electrolyte Li ₇ La ₃ Zr ₂ O ₁₂ . <i>Chemistry of Materials</i> , 2020 , 32, 1876-1886	9.6	15
76	Descriptors for Electron and Hole Charge Carriers in Metal Oxides. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 438-444	6.4	15
75	Local Charge Inhomogeneity and Lithium Distribution in the Superionic Argyrodites LiPSX (X = Cl, Br, I). <i>Inorganic Chemistry</i> , 2020 , 59, 11009-11019	5.1	27
74	Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O ₂ (NMC) Battery Cathodes. <i>Chemistry of Materials</i> , 2020 , 32, 7542-7550	9.6	14
73	Exploiting cationic vacancies for increased energy densities in dual-ion batteries. <i>Energy Storage Materials</i> , 2020 , 25, 154-163	19.4	14
72	Highly Anisotropic Thermal Transport in LiCoO. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 5552-5556.4	6.4	12
71	Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials. <i>Physical Review B</i> , 2019 , 99,	3.3	33
70	crystal-torture: A crystal tortuosity module. <i>Journal of Open Source Software</i> , 2019 , 4, 1306	5.2	1
69	pyscses: a PYthon Space-Charge Site-Explicit Solver. <i>Journal of Open Source Software</i> , 2019 , 4, 1209	5.2	

68	An introduction to classical molecular dynamics simulation for experimental scattering users. <i>Journal of Applied Crystallography</i> , 2019 , 52, 665-668	3.8	0
67	Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications. <i>APL Materials</i> , 2019 , 7, 022509	5.7	12
66	Impact of Anion Vacancies on the Local and Electronic Structures of Iron-Based Oxyfluoride Electrodes. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 107-112	6.4	10
65	Lithium Intercalation in Anatase Titanium Vacancies and the Role of Local Anionic Environment. <i>Chemistry of Materials</i> , 2018 , 30, 3078-3089	9.6	32
64	The electrochemical storage mechanism in oxy-hydroxyfluorinated anatase for sodium-ion batteries. <i>Inorganic Chemistry Frontiers</i> , 2018 , 5, 1100-1106	6.8	5
63	Controlled hydroxy-fluorination reaction of anatase to promote Mg mobility in rechargeable magnesium batteries. <i>Chemical Communications</i> , 2018 , 54, 10080-10083	5.8	13
62	Interfacial strain effects on lithium diffusion pathways in the spinel solid electrolyte Li-doped MgAl ₂ O ₄ . <i>Physical Review Materials</i> , 2018 , 2,	3.2	10
61	Role of spin-orbit coupling in the electronic structure of IrO ₂ . <i>Physical Review Materials</i> , 2018 , 2,	3.2	9
60	pylj: A teaching tool for classical atomistic simulation. <i>The Journal of Open Source Education</i> , 2018 , 1, 19	1.2	2
59	Inducing High Ionic Conductivity in the Lithium Superionic Argyrodites LiPGe SI for All-Solid-State Batteries. <i>Journal of the American Chemical Society</i> , 2018 , 140, 16330-16339	16.4	205
58	Self-Consistent Hybrid Functional Calculations: Implications for Structural, Electronic, and Optical Properties of Oxide Semiconductors. <i>Nanoscale Research Letters</i> , 2017 , 12, 19	5	31
57	A Reversible Phase Transition for Sodium Insertion in Anatase TiO ₂ . <i>Chemistry of Materials</i> , 2017 , 29, 1836-1844	9.6	54
56	Lattice-geometry effects in garnet solid electrolytes: a lattice-gas Monte Carlo simulation study. <i>Royal Society Open Science</i> , 2017 , 4, 170824	3.3	35
55	Reversible magnesium and aluminium ions insertion in cation-deficient anatase TiO. <i>Nature Materials</i> , 2017 , 16, 1142-1148	27	270
54	lattice_mc: A Python Lattice-Gas Monte Carlo Module. <i>Journal of Open Source Software</i> , 2017 , 2, 247	5.2	2
53	bsym: A basic symmetry module. <i>Journal of Open Source Software</i> , 2017 , 2, 370	5.2	1
52	Stability of the M2 phase of vanadium dioxide induced by coherent epitaxial strain. <i>Physical Review B</i> , 2016 , 94,	3.3	51
51	Sparse Cyclic Excitations Explain the Low Ionic Conductivity of Stoichiometric Li ₇ La ₃ Zr ₂ O ₁₂ . <i>Physical Review Letters</i> , 2016 , 116, 135901	7.4	41

50	Influence of Rotational Distortions on Li ⁺ - and Na ⁺ -Intercalation in Anti-NASICON Fe ₂ (MoO ₄) ₃ . <i>Chemistry of Materials</i> , 2016 , 28, 4492-4500	9.6	29
49	Lithium-ion conductivity in Li ₆ Y(BO ₃) ₃ : a thermally and electrochemically robust solid electrolyte. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 6972-6979	13	9
48	Variation in surface energy and reduction drive of a metal oxide lithium-ion anode with stoichiometry: a DFT study of lithium titanate spinel surfaces. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 17180-17192	13	16
47	Two-Dimensional Nanosystems. <i>Series in Materials Science and Engineering</i> , 2016 , 83-111		
46	Density functional theory screening of gas-treatment strategies for stabilization of high energy-density lithium metal anodes. <i>Journal of Power Sources</i> , 2015 , 296, 150-161	8.9	49
45	The electronic structure of silver orthophosphate: experiment and theory. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 6092-6099	13	18
44	Relationships between atomic diffusion mechanisms and ensemble transport coefficients in crystalline polymorphs. <i>Physical Review Letters</i> , 2014 , 112, 145901	7.4	30
43	Understanding the electronic structure of IrO ₂ using hard-X-ray photoelectron spectroscopy and density-functional theory. <i>Physical Review Letters</i> , 2014 , 112, 117601	7.4	80
42	Molecular dynamics simulation of ionic transport at coherent interfaces in fluorite heterostructures. <i>Physical Review B</i> , 2014 , 89,	3.3	4
41	Analysis of Intrinsic Defects in CeO ₂ Using a Koopmans-Like GGA+U Approach. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 2443-2452	3.8	125
40	Absence of a space-charge-derived enhancement of ionic conductivity in α -heterostructured 7H- and 9R-Agl. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 275303	1.8	9
39	Lithium intercalation into TiO ₂ (B): A comparison of LDA, GGA, and GGA+U density functional calculations. <i>Physical Review B</i> , 2012 , 86,	3.3	42
38	Role of Lithium Ordering in the Li _x TiO ₂ Anatase - β -titanate Phase Transition. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 1657-1661	6.4	38
37	The origin of the enhanced oxygen storage capacity of Ce(1-x)(Pd/Pt)(x)O ₂ . <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 4279-84	3.6	74
36	Effects of lattice polarity on interfacial space charges and defect disorder in ionically conducting AgI heterostructures. <i>Physical Review Letters</i> , 2011 , 107, 206102	7.4	12
35	Chemical bonding in copper-based transparent conducting oxides: CuMO ₂ (M = In, Ga, Sc). <i>Journal of Physics Condensed Matter</i> , 2011 , 23, 334201	1.8	22
34	Comment on α -Generalized Gradient Approximation +U Study for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxide \square <i>Japanese Journal of Applied Physics</i> , 2011 , 50, 069101	1.4	1
33	Comment on α -Generalized Gradient Approximation +U Study for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxide \square <i>Japanese Journal of Applied Physics</i> , 2011 , 50, 069101	1.4	

32	Understanding conductivity anomalies in Cu(I)-based delafossite transparent conducting oxides: Theoretical insights. <i>Journal of Chemical Physics</i> , 2010 , 132, 024707	3.9	93
31	GGA+U description of lithium intercalation into anatase TiO ₂ . <i>Physical Review B</i> , 2010 , 82,	3.3	93
30	Understanding conductivity in SrCu ₂ O ₂ : stability, geometry and electronic structure of intrinsic defects from first principles. <i>Journal of Materials Chemistry</i> , 2010 , 20, 1086-1096		39
29	First-principles study of epitaxial strain as a method of B ₄ -BCT stabilization in ZnO, ZnS, and CdS. <i>Physical Review B</i> , 2010 , 82,	3.3	27
28	Intrinsic n-type Defect Formation in TiO ₂ : A Comparison of Rutile and Anatase from GGA+U Calculations. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 2321-2328	3.8	326
27	A GGA+U study of the reduction of ceria surfaces and their partial reoxidation through NO ₂ adsorption. <i>Molecular Simulation</i> , 2009 , 35, 577-583	2	30
26	Preferential stability of the d-BCT phase in ZnO thin films. <i>Physical Review B</i> , 2009 , 80,	3.3	38
25	Polaronic trapping of electrons and holes by native defects in anatase TiO ₂ . <i>Physical Review B</i> , 2009 , 80,	3.3	222
24	Comparative study of bandwidths in copper delafossites from x-ray emission spectroscopy. <i>Physical Review B</i> , 2009 , 80,	3.3	33
23	A Density Functional Theory + U Study of Oxygen Vacancy Formation at the (110), (100), (101), and (001) Surfaces of Rutile TiO ₂ . <i>Journal of Physical Chemistry C</i> , 2009 , 113, 7322-7328	3.8	192
22	Reactivity on the (110) Surface of Ceria: A GGA+U Study of Surface Reduction and the Adsorption of CO and NO ₂ . <i>Journal of Physical Chemistry C</i> , 2009 , 113, 11095-11103	3.8	63
21	Acceptor levels in p-type Cu(2)O: rationalizing theory and experiment. <i>Physical Review Letters</i> , 2009 , 103, 096405	7.4	237
20	Small polarons in Nb- and Ta-doped rutile and anatase TiO ₂ . <i>Journal of Materials Chemistry</i> , 2009 , 19, 5175		143
19	Modeling the polaronic nature of p-type defects in Cu ₂ O: the failure of GGA and GGA + U. <i>Journal of Chemical Physics</i> , 2009 , 131, 124703	3.9	113
18	X-ray spectroscopic study of the electronic structure of CuCrO ₂ . <i>Physical Review B</i> , 2009 , 79,	3.3	82
17	Effect of Cr substitution on the electronic structure of CuAl _{1-x} Cr _x O ₂ . <i>Physical Review B</i> , 2009 , 79,	3.3	102
16	The Use of the "U" Correction in Describing Defect States at Metal Oxide Surfaces: Oxygen Vacancies on CeO ₂ and TiO ₂ , and Li-doping of MgO. <i>E-Journal of Surface Science and Nanotechnology</i> , 2009 , 7, 389-394	0.7	24
15	Competing Defect Mechanisms and Hydrogen Adsorption on Li-Doped MgO Low Index Surfaces: A DFT+U Study. <i>E-Journal of Surface Science and Nanotechnology</i> , 2009 , 7, 395-404	0.7	9

14	An ab initio Study of Reduction of V ₂ O ₅ through the Formation of Oxygen Vacancies and Li Intercalation. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 9903-9911	3.8	181
13	Molecular dynamics simulation of the six- to four-coordinate pressure-driven transition in MX nanocrystals: Mechanistic consequences of Σ grain boundaries in the high-pressure starting structure. <i>Physical Review B</i> , 2008 , 78,	3.3	10
12	A molecular dynamics study of structural relaxation in tetrahedrally coordinated nanocrystals. <i>Physical Chemistry Chemical Physics</i> , 2007 , 9, 2355-61	3.6	18
11	Pressure-Driven Phase Transitions in Crystalline Nanoparticles: Surface Effects on Hysteresis. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 6724-6731	3.8	22
10	Surface Sensitivity in Lithium-Doping of MgO: A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 7971-7979	3.8	91
9	A DFT+U description of oxygen vacancies at the TiO ₂ rutile (110) surface. <i>Surface Science</i> , 2007 , 601, 5034-5041	1.8	410
8	Simulation of the pressure-driven wurtzite to rock salt phase transition in nanocrystals. <i>Physical Chemistry Chemical Physics</i> , 2006 , 8, 3304-13	3.6	26
7	An atomistic MD simulation and pair-distribution-function study of disorder and reactivity of alpha-AlF ₃ nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2006 , 8, 5045-55	3.6	38
6	Ion mobilities and microscopic dynamics in liquid (Li,K)Cl. <i>Journal of Chemical Physics</i> , 2004 , 120, 1402-133.9		70
5	Pressure-Driven Sphalerite to Rock Salt Transition in Ionic Nanocrystals: A Simulation Study. <i>Nano Letters</i> , 2004 , 4, 1581-1585	11.5	34
4	Pushing the boundaries of lithium battery research with atomistic modelling on different scales. <i>Progress in Energy</i> ,	7.7	2
3	From Atoms to Cells: Multiscale Modeling of Li _{Nix} MnyCozO ₂ Cathodes for Li-Ion Batteries. <i>ACS Energy Letters</i> , 108-122	20.1	4
2	Mechanistic Origin of Superionic Lithium Diffusion in Anion-Disordered Li ₆ PS ₅ X Argyrodites		3
1	Anharmonic lattice dynamics of superionic lithium nitride. <i>Journal of Materials Chemistry A</i> ,	13	1