# Benjamin J Morgan

## List of Publications by Citations



| | | | |
|---|---|---|---|
| 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 | A DFT+U description of oxygen vacancies at the TiO2 rutile (110) surface. *Surface Science*, **2007**, 601, 5034-5041 | 1.8 | 410 |
| 84 | Intrinsic n-type Defect Formation in TiO2: A Comparison of Rutile and Anatase from GGA+U Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 2321-2328 | 3.8 | 326 |
| 83 | Reversible magnesium and aluminium ions insertion in cation-deficient anatase TiO. *Nature Materials*, **2017**, 16, 1142-1148 | 27 | 270 |
| 82 | Acceptor levels in p-type Cu(2)O: rationalizing theory and experiment. *Physical Review Letters*, **2009** , 103, 096405 | 7.4 | 237 |
| 81 | Polaronic trapping of electrons and holes by native defects in anatase TiO2. *Physical Review B*, **2009** , 80, | 3.3 | 222 |
| 80 | Inducing High Ionic Conductivity in the Lithium Superionic Argyrodites LiPGe SI for All-Solid-State Batteries. *Journal of the American Chemical Society*, **2018**, 140, 16330-16339 | 16.4 | 205 |
| 79 | A Density Functional Theory + U Study of Oxygen Vacancy Formation at the (110), (100), (101), and (001) Surfaces of Rutile TiO2. *Journal of Physical Chemistry C*, **2009**, 113, 7322-7328 | 3.8 | 192 |
| 78 | An ab initio Study of Reduction of V2O5 through the Formation of Oxygen Vacancies and Li Intercalation. *Journal of Physical Chemistry C*, **2008**, 112, 9903-9911 | 3.8 | 181 |
| 77 | Small polarons in Nb- and Ta-doped rutile and anatase TiO2. *Journal of Materials Chemistry*, **2009**, 19, 5175 | | 143 |
| 76 | Analysis of Intrinsic Defects in CeO2 Using a Koopmans-Like GGA+U Approach. *Journal of Physical Chemistry C*, **2012**, 116, 2443-2452 | 3.8 | 125 |
| 75 | Modeling the polaronic nature of p-type defects in Cu2O: the failure of GGA and GGA + U. *Journal of Chemical Physics*, **2009**, 131, 124703 | 3.9 | 113 |
| 74 | Effect of Cr substitution on the electronic structure of CuAl1⊠CrxO2. *Physical Review B*, **2009**, 79, | 3.3 | 102 |
| 73 | Understanding conductivity anomalies in Cu(I)-based delafossite transparent conducting oxides: Theoretical insights. *Journal of Chemical Physics*, **2010**, 132, 024707 | 3.9 | 93 |
| 72 | GGA+U description of lithium intercalation into anatase TiO2. *Physical Review B*, **2010**, 82, | 3.3 | 93 |
| 71 | Surface Sensitivity in Lithium-Doping of MgO:  A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. *Journal of Physical Chemistry C*, **2007**, 111, 7971-7979 | 3.8 | 91 |
| 70 | X-ray spectroscopic study of the electronic structure of CuCrO2. *Physical Review B*, **2009**, 79, | 3.3 | 82 |
| 69 | Understanding the electronic structure of IrO2 using hard-X-ray photoelectron spectroscopy and density-functional theory. *Physical Review Letters*, **2014**, 112, 117601 | 7.4 | 80 |

| | | | |
|---|---|---|---|
| 68 | The origin of the enhanced oxygen storage capacity of Ce(1-x)(Pd/Pt)(x)O2. *Physical Chemistry Chemical Physics*, **2011**, 13, 4279-84 | 3.6 | 74 |
| 67 | Ion mobilities and microscopic dynamics in liquid (Li,K)Cl. *Journal of Chemical Physics*, **2004**, 120, 1402-13 | 3.9 | 70 |
| 66 | Reactivity on the (110) Surface of Ceria: A GGA+U Study of Surface Reduction and the Adsorption of CO and NO2. *Journal of Physical Chemistry C*, **2009**, 113, 11095-11103 | 3.8 | 63 |
| 65 | A Reversible Phase Transition for Sodium Insertion in Anatase TiO2. *Chemistry of Materials*, **2017**, 29, 1836-1844 | 9.6 | 54 |
| 64 | Stability of the M2 phase of vanadium dioxide induced by coherent epitaxial strain. *Physical Review B*, **2016**, 94, | 3.3 | 51 |
| 63 | Density functional theory screening of gas-treatment strategies for stabilization of high energy-density lithium metal anodes. *Journal of Power Sources*, **2015**, 296, 150-161 | 8.9 | 49 |
| 62 | Lithium intercalation into TiO2(B): A comparison of LDA, GGA, and GGA+U density functional calculations. *Physical Review B*, **2012**, 86, | 3.3 | 42 |
| 61 | Sparse Cyclic Excitations Explain the Low Ionic Conductivity of Stoichiometric Li_{7}La_{3}Zr_{2}O_{12}. *Physical Review Letters*, **2016**, 116, 135901 | 7.4 | 41 |
| 60 | Understanding conductivity in SrCu2O2: stability, geometry and electronic structure of intrinsic defects from first principles. *Journal of Materials Chemistry*, **2010**, 20, 1086-1096 | | 39 |
| 59 | Role of Lithium Ordering in the LixTiO2 Anatase -Titanate Phase Transition. *Journal of Physical Chemistry Letters*, **2011**, 2, 1657-1661 | 6.4 | 38 |
| 58 | Preferential stability of the d-BCT phase in ZnO thin films. *Physical Review B*, **2009**, 80, | 3.3 | 38 |
| 57 | An atomistic MD simulation and pair-distribution-function study of disorder and reactivity of alpha-AlF3 nanoparticles. *Physical Chemistry Chemical Physics*, **2006**, 8, 5045-55 | 3.6 | 38 |
| 56 | Lattice-geometry effects in garnet solid electrolytes: a lattice-gas Monte Carlo simulation study. *Royal Society Open Science*, **2017**, 4, 170824 | 3.3 | 35 |
| 55 | Pressure-Driven Sphalerite to Rock Salt Transition in Ionic Nanocrystals: A Simulation Study. *Nano Letters*, **2004**, 4, 1581-1585 | 11.5 | 34 |
| 54 | Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials. *Physical Review B*, **2019**, 99, | 3.3 | 33 |
| 53 | Comparative study of bandwidths in copper delafossites from x-ray emission spectroscopy. *Physical Review B*, **2009**, 80, | 3.3 | 33 |
| 52 | Lithium Intercalation in Anatase Titanium Vacancies and the Role of Local Anionic Environment. *Chemistry of Materials*, **2018**, 30, 3078-3089 | 9.6 | 32 |
| 51 | Self-Consistent Hybrid Functional Calculations: Implications for Structural, Electronic, and Optical Properties of Oxide Semiconductors. *Nanoscale Research Letters*, **2017**, 12, 19 | 5 | 31 |

| | | | |
|---|---|---|---|
| 50 | Relationships between atomic diffusion mechanisms and ensemble transport coefficients in crystalline polymorphs. *Physical Review Letters*, **2014**, 112, 145901 | 7.4 | 30 |
| 49 | A GGA+U study of the reduction of ceria surfaces and their partial reoxidation through NO2 adsorption. *Molecular Simulation*, **2009**, 35, 577-583 | 2 | 30 |
| 48 | Influence of Rotational Distortions on Li+- and Na+-Intercalation in Anti-NASICON Fe2(MoO4)3. *Chemistry of Materials*, **2016**, 28, 4492-4500 | 9.6 | 29 |
| 47 | First-principles study of epitaxial strain as a method of B4-βCT stabilization in ZnO, ZnS, and CdS. *Physical Review B*, **2010**, 82, | 3.3 | 27 |
| 46 | Local Charge Inhomogeneity and Lithium Distribution in the Superionic Argyrodites LiPSX (X = Cl, Br, I). *Inorganic Chemistry*, **2020**, 59, 11009-11019 | 5.1 | 27 |
| 45 | Simulation of the pressure-driven wurtzite to rock salt phase transition in nanocrystals. *Physical Chemistry Chemical Physics*, **2006**, 8, 3304-13 | 3.6 | 26 |
| 44 | The Use of the “+U” Correction in Describing Defect States at Metal Oxide Surfaces: Oxygen Vacancies on CeO2 and TiO2, and Li-doping of MgO. *E-Journal of Surface Science and Nanotechnology*, **2009**, 7, 389-394 | 0.7 | 24 |
| 43 | Evidence for a Solid-Electrolyte Inductive Effect in the Superionic Conductor LiGeSnPS. *Journal of the American Chemical Society*, **2020**, 142, 21210-21219 | 16.4 | 23 |
| 42 | Chemical bonding in copper-based transparent conducting oxides: CuMO2 (M = In, Ga, Sc). *Journal of Physics Condensed Matter*, **2011**, 23, 334201 | 1.8 | 22 |
| 41 | Pressure-Driven Phase Transitions in Crystalline Nanoparticles: Surface Effects on Hysteresis. *Journal of Physical Chemistry C*, **2007**, 111, 6724-6731 | 3.8 | 22 |
| 40 | Mechanistic Origin of Superionic Lithium Diffusion in Anion-Disordered LiPS Argyrodites. *Chemistry of Materials*, **2021**, 33, 2004-2018 | 9.6 | 21 |
| 39 | The electronic structure of silver orthophosphate: experiment and theory. *Journal of Materials Chemistry A*, **2014**, 2, 6092-6099 | 13 | 18 |
| 38 | A molecular dynamics study of structural relaxation in tetrahedrally coordinated nanocrystals. *Physical Chemistry Chemical Physics*, **2007**, 9, 2355-61 | 3.6 | 18 |
| 37 | Variation in surface energy and reduction drive of a metal oxide lithium-ion anode with stoichiometry: a DFT study of lithium titanate spinel surfaces. *Journal of Materials Chemistry A*, **2016**, 4, 17180-17192 | 13 | 16 |
| 36 | Native Defects and Their Doping Response in the Lithium Solid Electrolyte Li7La3Zr2O12. *Chemistry of Materials*, **2020**, 32, 1876-1886 | 9.6 | 15 |
| 35 | Descriptors for Electron and Hole Charge Carriers in Metal Oxides. *Journal of Physical Chemistry Letters*, **2020**, 11, 438-444 | 6.4 | 15 |
| 34 | Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O2 (NMC) Battery Cathodes. *Chemistry of Materials*, **2020**, 32, 7542-7550 | 9.6 | 14 |
| 33 | Exploiting cationic vacancies for increased energy densities in dual-ion batteries. *Energy Storage Materials*, **2020**, 25, 154-163 | 19.4 | 14 |

| | | | |
|---|---|---|---|
| 32 | Atomic Insights into Aluminium-Ion Insertion in Defective Anatase for Batteries. *Angewandte Chemie - International Edition*, **2020**, 59, 19247-19253 | 16.4 | 13 |
| 31 | Controlled hydroxy-fluorination reaction of anatase to promote Mg mobility in rechargeable magnesium batteries. *Chemical Communications*, **2018**, 54, 10080-10083 | 5.8 | 13 |
| 30 | Highly Anisotropic Thermal Transport in LiCoO. *Journal of Physical Chemistry Letters*, **2019**, 10, 5552-5556 | 6.4 | 12 |
| 29 | Effects of lattice polarity on interfacial space charges and defect disorder in ionically conducting AgI heterostructures. *Physical Review Letters*, **2011**, 107, 206102 | 7.4 | 12 |
| 28 | Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications. *APL Materials*, **2019**, 7, 022509 | 5.7 | 12 |
| 27 | Molecular dynamics simulation of the six- to four-coordinate pressure-driven transition in MX nanocrystals: Mechanistic consequences of Σ3 grain boundaries in the high-pressure starting structure. *Physical Review B*, **2008**, 78, | 3.3 | 10 |
| 26 | Interfacial strain effects on lithium diffusion pathways in the spinel solid electrolyte Li-doped MgAl2O4. *Physical Review Materials*, **2018**, 2, | 3.2 | 10 |
| 25 | Impact of Anion Vacancies on the Local and Electronic Structures of Iron-Based Oxyfluoride Electrodes. *Journal of Physical Chemistry Letters*, **2019**, 10, 107-112 | 6.4 | 10 |
| 24 | Lithium-ion conductivity in Li6Y(BO3)3: a thermally and electrochemically robust solid electrolyte. *Journal of Materials Chemistry A*, **2016**, 4, 6972-6979 | 13 | 9 |
| 23 | Absence of a space-charge-derived enhancement of ionic conductivity in [illegible]heterostructured 7H- and 9R-AgI. *Journal of Physics Condensed Matter*, **2012**, 24, 275303 | 1.8 | 9 |
| 22 | Role of spin-orbit coupling in the electronic structure of IrO2. *Physical Review Materials*, **2018**, 2, | 3.2 | 9 |
| 21 | Competing Defect Mechanisms and Hydrogen Adsorption on Li-Doped MgO Low Index Surfaces: A DFT+U Study. *E-Journal of Surface Science and Nanotechnology*, **2009**, 7, 395-404 | 0.7 | 9 |
| 20 | The electrochemical storage mechanism in oxy-hydroxyfluorinated anatase for sodium-ion batteries. *Inorganic Chemistry Frontiers*, **2018**, 5, 1100-1106 | 6.8 | 5 |
| 19 | Molecular dynamics simulation of ionic transport at coherent interfaces in fluorite heterostructures. *Physical Review B*, **2014**, 89, | 3.3 | 4 |
| 18 | From Atoms to Cells: Multiscale Modeling of LiNixMnyCozO2 Cathodes for Li-Ion Batteries. *ACS Energy Letters*,108-122 | 20.1 | 4 |
| 17 | Mechanistic Origin of Superionic Lithium Diffusion in Anion-Disordered Li6PS5X Argyrodites | | 3 |
| 16 | Low-cost descriptors of electrostatic and electronic contributions to anion redox activity in batteries. *IOP SciNotes*, **2020**, 1, 024805 | 1.2 | 3 |
| 15 | Pushing the boundaries of lithium battery research with atomistic modelling on different scales. *Progress in Energy*, | 7.7 | 2 |

| | | | |
|---|---|---|---|
| 14 | pylj: A teaching tool for classical atomistic simulation. *The Journal of Open Source Education*, **2018**, 1, 19 | 1.2 | 2 |
| 13 | lattice_mc: A Python Lattice-Gas Monte Carlo Module. *Journal of Open Source Software*, **2017**, 2, 247 | 5.2 | 2 |
| 12 | Understanding fast-ion conduction in solid electrolytes. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2021**, 379, 20190451 | 3 | 2 |
| 11 | Impact of Solution Chemistry on Growth and Structural Features of Mo-Substituted Spinel Iron Oxides. *Inorganic Chemistry*, **2021**, 60, 7217-7227 | 5.1 | 2 |
| 10 | Comment on Generalized Gradient Approximation +UStudy for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxide *Japanese Journal of Applied Physics*, **2011**, 50, 069101 | 1.4 | 1 |
| 9 | crystal-torture: A crystal tortuosity module. *Journal of Open Source Software*, **2019**, 4, 1306 | 5.2 | 1 |
| 8 | Anharmonic lattice dynamics of superionic lithium nitride. *Journal of Materials Chemistry A*, | 13 | 1 |
| 7 | bsym: A basic symmetry module. *Journal of Open Source Software*, **2017**, 2, 370 | 5.2 | 1 |
| 6 | Overscreening and Underscreening in Solid-Electrolyte Grain Boundary Space-Charge Layers. *Physical Review Letters*, **2021**, 127, 135502 | 7.4 | 1 |
| 5 | Atomic Insights into Aluminium-Ion Insertion in Defective Anatase for Batteries. *Angewandte Chemie*, **2020**, 132, 19409-19415 | 3.6 | 0 |
| 4 | An introduction to classical molecular dynamics simulation for experimental scattering users. *Journal of Applied Crystallography*, **2019**, 52, 665-668 | 3.8 | 0 |
| 3 | pyscses: a PYthon Space-Charge Site-Explicit Solver. *Journal of Open Source Software*, **2019**, 4, 1209 | 5.2 | |
| 2 | Two-Dimensional Nanosystems. *Series in Materials Science and Engineering*, **2016**, 83-111 | | |
| 1 | Comment on Generalized Gradient Approximation +UStudy for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxide *Japanese Journal of Applied Physics*, **2011**, 50, 069101 | 1.4 | |