# Benjamin J Morgan

List of Publications by Year
in descending order



| | | | |
|---|---|---|---|
| 85 papers | 5,312 citations | 101384 36 h-index | 82410 72 g-index |
| 102 all docs | 102 docs citations | 102 times ranked | 7610 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | A DFT+U description of oxygen vacancies at the TiO2 rutile (110) surface. Surface Science, 2007, 601, 5034-5041. | 0.8 | 475 |
| 2 | Intrinsic n-type Defect Formation in TiO<sub>2</sub>: A Comparison of Rutile and Anatase from GGA+U Calculations. Journal of Physical Chemistry C, 2010, 114, 2321-2328. | 1.5 | 367 |
| 3 | Reversible magnesium and aluminium ions insertion in cation-deficient anatase TiO2. Nature Materials, 2017, 16, 1142-1148. | 13.3 | 366 |
| 4 | Inducing High Ionic Conductivity in the Lithium Superionic Argyrodites Li<sub>6+x</sub>P<sub>1â€“x</sub>Ge<sub>x</sub>S<sub>5</sub>I for All-Solid-State Batteries. Journal of the American Chemical Society, 2018, 140, 16330-16339. | 6.6 | 331 |
| 5 | Acceptor Levels in ZnO from Hybrid Density Functional Energy Calculations: Validation for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-Type <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="bold">O</mml:mi></mml:math>: Rationalizing Theory and Experiment. Physical Review | 2.9 | 265 |
| 6 | Polaronic trapping of electrons and holes by native defects in anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2009, 80, . | 1.1 | 247 |
| 7 | A Density Functional Theory + U Study of Oxygen Vacancy Formation at the (110), (100), (101), and (001) Surfaces of Rutile TiO<sub>2</sub>. Journal of Physical Chemistry C, 2009, 113, 7322-7328. | 1.5 | 223 |
| 8 | An ab initio Study of Reduction of V<sub>2</sub>O<sub>5</sub> through the Formation of Oxygen Vacancies and Li Intercalation. Journal of Physical Chemistry C, 2008, 112, 9903-9911. | 1.5 | 213 |
| 9 | Small polarons in Nb- and Ta-doped rutile and anatase TiO2. Journal of Materials Chemistry, 2009, 19, 5175. | 6.7 | 154 |
| 10 | Analysis of Intrinsic Defects in CeO<sub>2</sub> Using a Koopmans-Like GGA+U Approach. Journal of Physical Chemistry C, 2012, 116, 2443-2452. | 1.5 | 144 |
| 11 | Modeling the polaronic nature of p-type defects in Cu2O: The failure of GGA and GGA+U. Journal of Chemical Physics, 2009, 131, 124703. | 1.2 | 124 |
| 12 | Effect of Cr substitution on the electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CuAl</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn> Physical Review B, 2009, 79, . | 1.1 | 116 |
| 13 | Understanding the Electronic Structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>IrO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Hard-X-ray Photoelectron Spectroscopy and Density-Functional Theory. Physical Review Letters, 2014, 112, 117601. | 2.9 | 107 |
| 14 | Understanding conductivity anomalies in CuI-based delafossite transparent conducting oxides: Theoretical insights. Journal of Chemical Physics, 2010, 132, 024707. | 1.2 | 101 |
| 15 | <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>GGA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> of lithium intercalation into anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2010, 82, . | 1.1 | 100 |
| 16 | Surface Sensitivity in Lithium-Doping of MgO:â€‰ A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. Journal of Physical Chemistry C, 2007, 111, 7971-7979. | 1.5 | 96 |
| 17 | X-ray spectroscopic study of the electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CuCrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2009, 79, . | 1.1 | 88 |
| 18 | The origin of the enhanced oxygen storage capacity of Ce1â^'x(Pd/Pt)xO2. Physical Chemistry Chemical Physics, 2011, 13, 4279. | 1.3 | 85 |

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|---|---|---|---|
| 19 | Ion mobilities and microscopic dynamics in liquid (Li,K)Cl. Journal of Chemical Physics, 2004, 120, 1402-1413. | 1.2 | 76 |
| 20 | A Reversible Phase Transition for Sodium Insertion in Anatase TiO<sub>2</sub>. Chemistry of Materials, 2017, 29, 1836-1844. | 3.2 | 68 |
| 21 | Reactivity on the (110) Surface of Ceria: A GGA+UStudy of Surface Reduction and the Adsorption of CO and NO<sub>2</sub>. Journal of Physical Chemistry C, 2009, 113, 11095-11103. | 1.5 | 66 |
| 22 | Mechanistic Origin of Superionic Lithium Diffusion in Anion-Disordered Li<sub>6</sub>PS<sub>5</sub>X Argyrodites. Chemistry of Materials, 2021, 33, 2004-2018. | 3.2 | 63 |
| 23 | Stability of the M2 phase of vanadium dioxide induced by coherent epitaxial strain. Physical Review B, 2016, 94, . | 1.1 | 62 |
| 24 | Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials. Physical Review B, 2019, 99, . | 1.1 | 60 |
| 25 | 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. | 4.0 | 57 |
| 26 | Sparse Cyclic Excitations Explain the Low Ionic Conductivity of Stoichiometric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Li</mml:mi></mml:mrow><mml:mrow><mml:mn>7</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O. Physical Review Letters, 2016, 116, 135901. | 2.9 | 57 |
| 27 | Local Charge Inhomogeneity and Lithium Distribution in the Superionic Argyrodites Li<sub>6</sub>PS<sub>5</sub>X (X = Cl, Br, I). Inorganic Chemistry, 2020, 59, 11009-11019. | 1.9 | 56 |
| 28 | Lithium intercalation into TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(B): A comparison of LDA, GGA, and GGA+<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>density functional calculations. Physical Review B, 2012, 86, . | 1.1 | 52 |
| 29 | Lattice-geometry effects in garnet solid electrolytes: a lattice-gas Monte Carlo simulation study. Royal Society Open Science, 2017, 4, 170824. | 1.1 | 50 |
| 30 | Lithium Intercalation in Anatase Titanium Vacancies and the Role of Local Anionic Environment. Chemistry of Materials, 2018, 30, 3078-3089. | 3.2 | 49 |
| 31 | Evidence for a Solid-Electrolyte Inductive Effect in the Superionic Conductor Li<sub>10</sub>Ge<sub>1â€“x</sub>Sn<sub>x</sub>P<sub>2</sub>S<sub>12</sub>. Journal of the American Chemical Society, 2020, 142, 21210-21219. | 6.6 | 43 |
| 32 | Understanding conductivity in SrCu<sub>2</sub>O<sub>2</sub>: stability, geometry and electronic structure of intrinsic defects from first principles. Journal of Materials Chemistry, 2010, 20, 1086-1096. | 6.7 | 42 |
| 33 | Preferential stability of the d-BCT phase in ZnO thin films. Physical Review B, 2009, 80, . | 1.1 | 41 |
| 34 | Role of Lithium Ordering in the Li<sub>x</sub>TiO<sub>2</sub> Anatase â†' Titanate Phase Transition. Journal of Physical Chemistry Letters, 2011, 2, 1657-1661. | 2.1 | 41 |
| 35 | An atomistic MD simulation and pair-distribution-function study of disorder and reactivity of Î±-AlF3nanoparticles. Physical Chemistry Chemical Physics, 2006, 8, 5045-5055. | 1.3 | 40 |
| 36 | Native Defects and Their Doping Response in the Lithium Solid Electrolyte Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub>. Chemistry of Materials, 2020, 32, 1876-1886. | 3.2 | 39 |

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|---|---|---|---|
| 37 | Influence of Rotational Distortions on Li<sup>+</sup>- and Na<sup>+</sup>-Intercalation in Anti-NASICON Fe<sub>2</sub>(MoO<sub>4</sub>)<sub>3</sub>. Chemistry of Materials, 2016, 28, 4492-4500. | 3.2 | 38 |
| 38 | Comparative study of bandwidths in copper delafossites from x-ray emission spectroscopy. Physical Review B, 2009, 80, . | 1.1 | 36 |
| 39 | Pressure-Driven Sphalerite to Rock Salt Transition in Ionic Nanocrystals:â€‰ A Simulation Study. Nano Letters, 2004, 4, 1581-1585. | 4.5 | 34 |
| 40 | Self-Consistent Hybrid Functional Calculations: Implications for Structural, Electronic, and Optical Properties of Oxide Semiconductors. Nanoscale Research Letters, 2017, 12, 19. | 3.1 | 34 |
| 41 | Relationships between Atomic Diffusion Mechanisms and Ensemble Transport Coefficients in Crystalline Polymorphs. Physical Review Letters, 2014, 112, 145901. | 2.9 | 32 |
| 42 | A GGA+Ustudy of the reduction of ceria surfaces and their partial reoxidation through NO<sub>2</sub>adsorption. Molecular Simulation, 2009, 35, 577-583. | 0.9 | 31 |
| 43 | Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O<sub>2</sub> (NMC) Battery Cathodes. Chemistry of Materials, 2020, 32, 7542-7550. | 3.2 | 28 |
| 44 | Simulation of the pressure-driven wurtzite to rock salt phase transition in nanocrystals. Physical Chemistry Chemical Physics, 2006, 8, 3304. | 1.3 | 27 |
| 45 | First-principles study of epitaxial strain as a method of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>B</mml:mtext><mml:mn>4</mml:mn><mml:mo>â†’</mml:mo><mml:mtext>B</mml:mtext> in ZnO, ZnS, and CdS. Physical Review B, 2010, 82, . | 1.1 | 27 |
| 46 | Chemical bonding in copper-based transparent conducting oxides: CuMO<sub>2</sub>(M = In, Ga, Sc). Journal of Physics Condensed Matter, 2011, 23, 334201. | 0.7 | 25 |
| 47 | The Use of the “+U” Correction in Describing Defect States at Metal Oxide Surfaces: Oxygen Vacancies on CeO<sub>2</sub> and TiO<sub>2</sub>, and Li-doping of MgO. E-Journal of Surface Science and Nanotechnology, 2009, 7, 389-394. | 0.1 | 25 |
| 48 | Pressure-Driven Phase Transitions in Crystalline Nanoparticles:â€‰ Surface Effects on Hysteresis. Journal of Physical Chemistry C, 2007, 111, 6724-6731. | 1.5 | 24 |
| 49 | Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications. APL Materials, 2019, 7, . | 2.2 | 23 |
| 50 | 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. | 5.2 | 23 |
| 51 | Descriptors for Electron and Hole Charge Carriers in Metal Oxides. Journal of Physical Chemistry Letters, 2020, 11, 438-444. | 2.1 | 22 |
| 52 | Atomic Insights into Aluminiumâ€‐ion Insertion in Defective Anatase for Batteries. Angewandte Chemie - International Edition, 2020, 59, 19247-19253. | 7.2 | 22 |
| 53 | The electronic structure of silver orthophosphate: experiment and theory. Journal of Materials Chemistry A, 2014, 2, 6092-6099. | 5.2 | 21 |
| 54 | Exploiting cationic vacancies for increased energy densities in dual-ion batteries. Energy Storage Materials, 2020, 25, 154-163. | 9.5 | 20 |

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|---|---|---|---|
| 55 | A molecular dynamics study of structural relaxation in tetrahedrally coordinated nanocrystals. Physical Chemistry Chemical Physics, 2007, 9, 2355. | 1.3 | 18 |
| 56 | Highly Anisotropic Thermal Transport in LiCoO<sub>2</sub>. Journal of Physical Chemistry Letters, 2019, 10, 5552-5556. | 2.1 | 17 |
| 57 | Impact of Anion Vacancies on the Local and Electronic Structures of Iron-Based Oxyfluoride Electrodes. Journal of Physical Chemistry Letters, 2019, 10, 107-112. | 2.1 | 16 |
| 58 | From Atoms to Cells: Multiscale Modeling of LiNi<sub>x</sub>Mn<sub>y</sub>Co<sub>z</sub>O<sub>2</sub> Cathodes for Li-Ion Batteries. ACS Energy Letters, 2022, 7, 108-122. | 8.8 | 16 |
| 59 | Effects of Lattice Polarity on Interfacial Space Charges and Defect Disorder in Ionically Conducting AgI Heterostructures. Physical Review Letters, 2011, 107, 206102. | 2.9 | 15 |
| 60 | Controlled hydroxy-fluorination reaction of anatase to promote Mg<sup>2+</sup> mobility in rechargeable magnesium batteries. Chemical Communications, 2018, 54, 10080-10083. | 2.2 | 15 |
| 61 | Role of spin-orbit coupling in the electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ir</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2018, 2, . | 0.9 | 14 |
| 62 | Lithium-ion conductivity in Li<sub>6</sub>Y(BO<sub>3</sub>)<sub>3</sub>: a thermally and electrochemically robust solid electrolyte. Journal of Materials Chemistry A, 2016, 4, 6972-6979. | 5.2 | 13 |
| 63 | Interfacial strain effects on lithium diffusion pathways in the spinel solid electrolyte Li-doped MgAl2O4. Physical Review Materials, 2018, 2, . | 0.9 | 13 |
| 64 | Understanding fast-ion conduction in solid electrolytes. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20190451. | 1.6 | 12 |
| 65 | Pushing the boundaries of lithium battery research with atomistic modelling on different scales. Progress in Energy, 2022, 4, 012002. | 4.6 | 12 |
| 66 | Molecular dynamics simulation of the six- to four-coordinate pressure-driven transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>M</mml:mi><mml:mi>X</mml:mi></mml:mrow></mml:math>nanocrystals: Mechanistic consequences of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>Î£</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>grain boundaries in the high-pressure starting structure. Physical Review B, 2008, 78, . | 1.1 | 10 |
| 67 | Absence of a space-charge-derived enhancement of ionic conductivity in Î² \| Î³- heterostructured 7H- and 9R-AgI. Journal of Physics Condensed Matter, 2012, 24, 275303. | 0.7 | 9 |
| 68 | 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. | 0.1 | 9 |
| 69 | Anharmonic lattice dynamics of superionic lithium nitride. Journal of Materials Chemistry A, 2022, 10, 2295-2304. | 5.2 | 9 |
| 70 | Overscreening and Underscreening in Solid-Electrolyte Grain Boundary Space-Charge Layers. Physical Review Letters, 2021, 127, 135502. | 2.9 | 7 |
| 71 | Hydride ion intercalation and conduction in the electride Sr<sub>3</sub>CrN<sub>3</sub>. Journal of Materials Chemistry C, 2022, 10, 6628-6633. | 2.7 | 6 |
| 72 | The electrochemical storage mechanism in oxy-hydroxyfluorinated anatase for sodium-ion batteries. Inorganic Chemistry Frontiers, 2018, 5, 1100-1106. | 3.0 | 5 |

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| 73 | Low-cost descriptors of electrostatic and electronic contributions to anion redox activity in batteries. IOP SciNotes, 2020, 1, 024805. | 0.4 | 5 |
| 74 | Molecular dynamics simulation of ionic transport at coherent interfaces in fluorite heterostructures. Physical Review B, 2014, 89, . | 1.1 | 4 |
| 75 | Impact of Solution Chemistry on Growth and Structural Features of Mo-Substituted Spinel Iron Oxides. Inorganic Chemistry, 2021, 60, 7217-7227. | 1.9 | 3 |
| 76 | crystal-torture: A crystal tortuosity module. Journal of Open Source Software, 2019, 4, 1306. | 2.0 | 3 |
| 77 | bsym: A basic symmetry module. Journal of Open Source Software, 2017, 2, 370. | 2.0 | 3 |
| 78 | An introduction to classical molecular dynamics simulation for experimental scattering users. Journal of Applied Crystallography, 2019, 52, 665-668. | 1.9 | 3 |
| 79 | pylj: A teaching tool for classical atomistic simulation. The Journal of Open Source Education, 2018, 1, 19. | 0.2 | 2 |
| 80 | lattice_mc: A Python Lattice-Gas Monte Carlo Module. Journal of Open Source Software, 2017, 2, 247. | 2.0 | 2 |
| 81 | Comment on â€œGeneralized Gradient Approximation +U Study for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxideâ€• Japanese Journal of Applied Physics, 2011, 50, 069101. | 0.8 | 1 |
| 82 | Atomic Insights into Aluminiumâ€‘Ion Insertion in Defective Anatase for Batteries. Angewandte Chemie, 2020, 132, 19409-19415. | 1.6 | 1 |
| 83 | Comment on â€œGeneralized Gradient Approximation +UStudy for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxideâ€• Japanese Journal of Applied Physics, 2011, 50, 069101. | 0.8 | 0 |
| 84 | Two-Dimensional Nanosystems. Series in Materials Science and Engineering, 2016, , 83-111. | 0.1 | 0 |
| 85 | pyscses: a PYthon Space-Charge Site-Explicit Solver. Journal of Open Source Software, 2019, 4, 1209. | 2.0 | 0 |