# Blas P Uberuaga

List of Publications by Year
in descending order



| 275 | 25,859 | 36203 | 6818 |
|---|---|---|---|
| papers | citations | 51 h-index | 155 g-index |

| 288 | 288 | 288 | 22166 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | The effect of Cr alloying on defect migration at Ni grain boundaries. Journal of Materials Science, 2022, 57, 10499-10516. | 1.7 | 5 |
| 2 | Machine learning in nuclear materials research. Current Opinion in Solid State and Materials Science, 2022, 26, 100975. | 5.6 | 42 |
| 3 | The mechanism behind the high radiation tolerance of Feâ€“Cr alloys. Journal of Applied Physics, 2022, 131, . | 1.1 | 4 |
| 4 | Surprisingly high irradiation-induced defect mobility in Fe3O4 as revealed through in situ transmission electron microscopy. Materials Characterization, 2022, 187, 111863. | 1.9 | 2 |
| 5 | Microstructural dependence of defect formation in iron-oxide thin films. Applied Surface Science, 2022, 589, 152844. | 3.1 | 2 |
| 6 | Be surface structures on W(110) and W(211): A DFT study. Acta Materialia, 2022, 235, 118012. | 3.8 | 2 |
| 7 | Adatom-Driven Oxygen Intermixing during the Deposition of Oxide Thin Films by Molecular Beam Epitaxy. Nano Letters, 2022, 22, 4963-4969. | 4.5 | 4 |
| 8 | Inversion, chemical complexity, and interstitial transport in spinels. Journal of the American Ceramic Society, 2021, 104, 2313-2324. | 1.9 | 2 |
| 9 | Accelerated Molecular Dynamics Methods for Long-Time Simulations inÂMaterials. Springer Series in Materials Science, 2021, , 137-156. | 0.4 | 2 |
| 10 | Accurately predicting optical properties of rare-earth, aluminate scintillators: influence of electronâ€“hole correlation. Journal of Materials Chemistry C, 2021, 9, 7292-7301. | 2.7 | 8 |
| 11 | Microstructural analysis of novel Gd2Ti2O7 thin films processed via sputter deposition. Materials and Design, 2021, 199, 109430. | 3.3 | 5 |
| 12 | Interplay between defect transport and cation spin frustration in corundum-structured oxides. Physical Review Materials, 2021, 5, . | 0.9 | 5 |
| 13 | Radiation-Enhanced Anion Transport in Hematite. Chemistry of Materials, 2021, 33, 2307-2318. | 3.2 | 7 |
| 14 | The role of cation ordering and disordering on mass transport in complex oxides. Current Opinion in Solid State and Materials Science, 2021, 25, 100899. | 5.6 | 11 |
| 15 | Neutron irradiation induced defects in oxides and their impact on the oxide properties. Journal of Applied Physics, 2021, 129, 215901. | 1.1 | 2 |
| 16 | Reduction of bright exciton lifetimes by radiation-induced disorder. Physical Review Materials, 2021, 5, . | 0.9 | 1 |
| 17 | Effects of Radiation-Induced Defects on Corrosion. Annual Review of Materials Research, 2021, 51, 293-328. | 4.3 | 27 |
| 18 | Barriers to carriers: faults and recombination in non-stoichiometric perovskite scintillators. Journal of Materials Science, 2021, 56, 15812-15823. | 1.7 | 0 |

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| 19 | Modeling Disorder in Pyrochlores and Other Anion-Deficient Fluorite Structural Derivative Oxides. Frontiers in Chemistry, 2021, 9, 712543. | 1.8 | 6 |
| 20 | Recent advances in the structure and dynamics of complex oxides, with a focus on fundamentals. Current Opinion in Solid State and Materials Science, 2021, 25, 100942. | 5.6 | 1 |
| 21 | A Machine Learning Approach for the Prediction of Formability and Thermodynamic Stability of Single and Double Perovskite Oxides. Chemistry of Materials, 2021, 33, 845-858. | 3.2 | 64 |
| 22 | Radiation Enhanced Anion Diffusion in Chromia. Journal of Physical Chemistry C, 2021, 125, 27820-27827. | 1.5 | 5 |
| 23 | Light-driven permanent transition from insulator to conductor. Physical Review B, 2021, 104, . | 1.1 | 6 |
| 24 | Critical Assessment of the Thermodynamics of Vacancy Formation in Fe<sub>2</sub>O<sub>3</sub> Using Hybrid Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 23988-24000. | 1.5 | 10 |
| 25 | Role of Symmetry, Geometry, and Termination Chemistry on Misfit Dislocation Patterns at Semicoherent Heterointerfaces. Matter, 2020, 2, 1324-1337. | 5.0 | 4 |
| 26 | A new mechanism for void-cascade interaction from nondestructive depth-resolved atomic-scale measurements of ion irradiationâ€“induced defects in Fe. Science Advances, 2020, 6, eaba8437. | 4.7 | 32 |
| 27 | A pathway to synthesizing single-crystal Fe and FeCr films. Surface and Coatings Technology, 2020, 403, 126346. | 2.2 | 6 |
| 28 | Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. ACS Applied Materials & Interfaces, 2020, 12, 46296-46305. | 4.0 | 19 |
| 29 | Prediction of structure and cation ordering in an ordered normal-inverse double spinel. Communications Materials, 2020, 1, . | 2.9 | 46 |
| 30 | In-situ re-crystallization of heavily-irradiated Gd2Ti2O7. Acta Materialia, 2020, 194, 403-411. | 3.8 | 7 |
| 31 | Anion order in oxysulfide perovskites: origins and implications. Npj Computational Materials, 2020, 6, . | 3.5 | 22 |
| 32 | Measurement and Simulation of Vacancy Formation in 2-MeV Self-irradiated Pure Fe. Jom, 2020, 72, 2436-2444. | 0.9 | 1 |
| 33 | Molecular Dynamics. , 2020, , 573-594. | | 6 |
| 34 | Role of electronic and magnetic interactions in defect formation and anomalous diffusion in Î´-Pu. Journal of Nuclear Materials, 2020, 532, 152027. | 1.3 | 7 |
| 35 | Spatially-varying inversion near grain boundaries in MgAl<sub>2</sub>O<sub>4</sub> spinel. RSC Advances, 2020, 10, 11737-11742. | 1.7 | 5 |
| 36 | Chemical manipulation of hydrogen induced high p-type and n-type conductivity in Ga2O3. Scientific Reports, 2020, 10, 6134. | 1.6 | 65 |

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| 37 | Accelerated Molecular Dynamics Methods in a Massively Parallel World. , 2020, , 1-28. | | 1 |
| 38 | Accelerated Molecular Dynamics Methods in a Massively Parallel World. , 2020, , 745-772. | | 3 |
| 39 | High-throughput investigation of the formation of double spinels. Journal of Materials Chemistry A, 2020, 8, 25756-25767. | 5.2 | 36 |
| 40 | Mapping Cation Disorder in Irradiated Gd<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> Pyrochlore by 4D-STEM. Microscopy and Microanalysis, 2019, 25, 1560-1561. | 0.2 | 4 |
| 41 | An Overview of Recent Standard and Accelerated Molecular Dynamics Simulations of Helium Behavior in Tungsten. Materials, 2019, 12, 2500. | 1.3 | 7 |
| 42 | Hydrogen interactions with low-index surface orientations of tungsten. Journal of Physics Condensed Matter, 2019, 31, 255002. | 0.7 | 12 |
| 43 | Semicoherent oxide heterointerfaces: Structure, properties, and implications. APL Materials, 2019, 7, . | 2.2 | 19 |
| 44 | Depth Resolved Measurements of Atomic Scale Defects in Ion Irradiated Fe Alloys. Microscopy and Microanalysis, 2019, 25, 1546-1547. | 0.2 | 1 |
| 45 | First-principles localized cluster expansion study of the kinetics of hydrogen diffusion in homogeneous and heterogeneous Fe-Cr alloys. Physical Review B, 2019, 99, . | 1.1 | 16 |
| 46 | Beyond Coherent Oxide Heterostructures: Atomicâ€Scale Structure of Misfit Dislocations. Advanced Theory and Simulations, 2019, 2, 1900078. | 1.3 | 13 |
| 47 | Ab initio based examination of the kinetics and thermodynamics of oxygen in Fe-Cr alloys. Physical Review B, 2019, 99, . | 1.1 | 7 |
| 48 | Atomistic modeling of out-of-pile xenon diffusion by vacancy clusters in UO2. Journal of Nuclear Materials, 2019, 520, 96-109. | 1.3 | 27 |
| 49 | Multifidelity Information Fusion with Machine Learning: A Case Study of Dopant Formation Energies in Hafnia. ACS Applied Materials & Interfaces, 2019, 11, 24906-24918. | 4.0 | 49 |
| 50 | Dissociated vacancies and screw dislocations in MgO and UO2: atomistic modeling and linear elasticity analysis. Scientific Reports, 2019, 9, 6499. | 1.6 | 4 |
| 51 | Massively enhanced ionic transport in irradiated crystalline pyrochlore. Journal of Materials Chemistry A, 2019, 7, 3917-3923. | 5.2 | 23 |
| 52 | The impact of chemical order on defect transport in mixed pyrochlores. Physical Chemistry Chemical Physics, 2019, 21, 5956-5965. | 1.3 | 5 |
| 53 | The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. Applied Sciences (Switzerland), 2019, 9, 5276. | 1.3 | 11 |
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| 55 | Potential benefit of amorphization in the retention of gaseous species in irradiated pyrochlores. Acta Materialia, 2019, 164, 250-260. | 3.8 | 10 |
| 56 | Distortion-stabilized ordered structures in A2BBâ€™O7 mixed pyrochlores. Npj Computational Materials, 2019, 5, . | 3.5 | 23 |
| 57 | In-situ irradiation tolerance investigation of high strength ultrafine tungsten-titanium carbide alloy. Acta Materialia, 2019, 164, 547-559. | 3.8 | 37 |
| 58 | A comprehensive computational study of adatom diffusion on the aluminum (1â€¯0â€¯0) surface. Computational Materials Science, 2019, 158, 353-358. | 1.4 | 9 |
| 59 | Influence of Chemistry and Misfit Dislocation Structure on Dopant Segregation at Complex Oxide Heterointerfaces. Advanced Theory and Simulations, 2019, 2, 1800095. | 1.3 | 8 |
| 60 | Structure and Mobility of Dissociated Vacancies at Twist Grain Boundaries and Screw Dislocations in Ionic Rocksalt Compounds. Chemistry of Materials, 2018, 30, 1980-1988. | 3.2 | 3 |
| 61 | Discovering mechanisms relevant for radiation damage evolution. Computational Materials Science, 2018, 147, 282-292. | 1.4 | 12 |
| 62 | Physics-informed machine learning for inorganic scintillator discovery. Journal of Chemical Physics, 2018, 148, 241729. | 1.2 | 28 |
| 63 | Role of Sink Density in Nonequilibrium Chemical Redistribution in Alloys. Physical Review Letters, 2018, 120, 106101. | 2.9 | 23 |
| 64 | Synthesis and characterization of dense Gd2Ti2O7 pyrochlore thin films deposited using RF magnetron sputtering. Solid State Ionics, 2018, 314, 36-40. | 1.3 | 3 |
| 65 | On the role of electro-migration in the evolution of radiation damage in nanostructured ionic materials. Electrochemistry Communications, 2018, 96, 47-52. | 2.3 | 4 |
| 66 | Accelerated Molecular Dynamics Methods in a Massively Parallel World. , 2018, , 1-28. | | 1 |
| 67 | Atomistic model of xenon gas bubble re-solution rate due to thermal spike in uranium oxide. Journal of Applied Physics, 2018, 124, . | 1.1 | 13 |
| 68 | Formation of helium-bubble networks in tungsten. Acta Materialia, 2018, 159, 46-50. | 3.8 | 35 |
| 69 | New helium bubble growth mode at a symmetric grain-boundary in tungsten: accelerated molecular dynamics study. Materials Research Letters, 2018, 6, 522-530. | 4.1 | 20 |
| 70 | Radiation Response and Recovery of Gd2Ti2Q7 Pyrochlore. Microscopy and Microanalysis, 2018, 24, 1956-1957. | 0.2 | 0 |
| 71 | Role of Multiple Charge States of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Ce</mml:mi></mml:math> in the Scintillation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi mathvariant="italic">AB</mml:mi><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math> | 1.5 | 15 |
| 72 | How relative defect migration energies drive contrasting temperature-dependent microstructural evolution in irradiated ceramics. Physical Review Materials, 2018, 2, . | 0.9 | 8 |

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| 75 | Synthesis of Hf8O7, a new binary hafnium oxide, at high pressures and high temperatures. High Pressure Research, 2017, 37, 147-158. | 0.4 | 3 |
| 76 | Temperature Dependence Discontinuity in the Stability of Manganese-Doped Ceria Nanocrystals. Crystal Growth and Design, 2017, 17, 446-453. | 1.4 | 10 |
| 77 | Using Machine Learning To Identify Factors That Govern Amorphization of Irradiated Pyrochlores. Chemistry of Materials, 2017, 29, 2574-2583. | 3.2 | 33 |
| 78 | Radiation Tolerant Interfaces: Influence of Local Stoichiometry at the Misfit Dislocation on Radiation Damage Resistance of Metal/Oxide Interfaces. Advanced Materials Interfaces, 2017, 4, 1700037. | 1.9 | 10 |
| 79 | Disorder-induced transition from grain boundary to bulk dominated ionic diffusion in pyrochlores. Nanoscale, 2017, 9, 6826-6836. | 2.8 | 8 |
| 80 | Cr incorporated phase transformation in Y2O3 under ion irradiation. Scientific Reports, 2017, 7, 40148. | 1.6 | 6 |
| 81 | Reduced grain boundary energies in rare-earth doped MgAl2O4 spinel and consequent grain growth inhibition. Journal of the European Ceramic Society, 2017, 37, 4043-4050. | 2.8 | 38 |
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| 84 | Evidence for percolation diffusion of cations and reordering in disordered pyrochlore from accelerated molecular dynamics. Nature Communications, 2017, 8, 618. | 5.8 | 28 |
| 85 | Onset conditions for flash sintering of UO2. Journal of Nuclear Materials, 2017, 493, 264-270. | 1.3 | 27 |
| 86 | The mobility of small vacancy/helium complexes in tungsten and its impact on retention in fusion-relevant conditions. Scientific Reports, 2017, 7, 2522. | 1.6 | 50 |
| 87 | Growth Rate Effects on the Formation of Dislocation Loops Around Deep Helium Bubbles in Tungsten. Fusion Science and Technology, 2017, 71, 1-6. | 0.6 | 20 |
| 88 | The Modern Temperature-Accelerated Dynamics Approach. Annual Review of Chemical and Biomolecular Engineering, 2016, 7, 87-110. | 3.3 | 45 |
| 89 | The effects of cationâ€“anion clustering on defect migration in MgAl<sub>2</sub>O<sub>4</sub>. Physical Chemistry Chemical Physics, 2016, 18, 19647-19654. | 1.3 | 12 |
| 90 | Improving the Thermodynamic Stability of Aluminate Spinel Nanoparticles with Rare Earths. Chemistry of Materials, 2016, 28, 5163-5171. | 3.2 | 27 |

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| 91 | The thermodynamic and kinetic interactions of He interstitial clusters with bubbles in W. Journal of Applied Physics, 2016, 119, . | 1.1 | 21 |
| 92 | Stabilization of MgAl2O4 spinel surfaces via doping. Surface Science, 2016, 649, 138-145. | 0.8 | 33 |
| 93 | Temperature dependence of the radiation tolerance of nanocrystalline pyrochlores A2Ti2O7 (AÂ=ÂGd, Ho) Tj ETQq1 1 0.784314 rgBT /C | 3.8 | 34 |
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| 99 | Interaction of small mobile stacking fault tetrahedra with free surfaces, dislocations, and interfaces in Cu and Cu-Nb. Physical Review B, 2016, 93, . | 1.1 | 28 |
| 100 | EfficientAbÂinitioModeling of Random Multicomponent Alloys. Physical Review Letters, 2016, 116, 105501. | 2.9 | 93 |
| 101 | Machine learning bandgaps of double perovskites. Scientific Reports, 2016, 6, 19375. | 1.6 | 354 |
| 102 | Irradiation-induced grain growth and defect evolution in nanocrystalline zirconia with doped grain boundaries. Physical Chemistry Chemical Physics, 2016, 18, 16921-16929. | 1.3 | 20 |
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| 110 | Band-Gap and Band-Edge Engineering of Multicomponent Garnet Scintillators from First Principles. Physical Review Applied, 2015, 4, . | 1.5 | 62 |
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| 112 | Thermally Induced Interdiffusion and Precipitation in a Ni/Ni<sub>3</sub>Al System. Materials Research Letters, 2015, 3, 169-176. | 4.1 | 5 |
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| 115 | Defect-interface interactions. Progress in Materials Science, 2015, 74, 125-210. | 16.0 | 450 |
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| 117 | Accelerated chemical aging of crystalline nuclear waste forms: A density functional theory study of 109<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si6.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cd</mml:mtext></mml:mrow><mml:mrow><mml:mi>x</mml:mi> xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si7.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ag</mml:mtext></mml:mrow><mml:mrow><mml:mn>. Nuclear Instruments & Methods in Physics Research B, 2015, 352, 130-134. | 0.6 | 0 |
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| 119 | Competing Kinetics and He Bubble Morphology in W. Physical Review Letters, 2015, 114, 105502. | 2.9 | 108 |
| 120 | Microstructure, chemistry and mechanical properties of Ni-based superalloy Rene N4 under irradiation at room temperature. Acta Materialia, 2015, 95, 357-365. | 3.8 | 46 |
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| 122 | Uranium vacancy mobility at the Î£5 symmetric tilt and Î£5 twist grain boundaries in UO2. Computational Materials Science, 2015, 108, 80-87. | 1.4 | 5 |
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| 125 | Effect of Cation Ordering on Oxygen Vacancy Diffusion Pathways in Double Perovskites. Chemistry of Materials, 2015, 27, 5020-5026. | 3.2 | 32 |
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| 131 | The relationship between grain boundary structure, defect mobility and grain boundary sink efficiency. Scientific Reports, 2015, 5, 9095. | 1.6 | 136 |
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| 133 | Cation ordering and effect of biaxial strain in double perovskite CsRbCaZnCl6. Journal of Applied Physics, 2015, 117, . | 1.1 | 8 |
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| 136 | Prediction of Irradiation Spectrum Effects in Pyrochlores. Jom, 2014, 66, 2578-2582. | 0.9 | 6 |
| 137 | Role of the interface on radiation damage in the SrTiO3/LaAlO3 heterostructure under Ne2+ ion irradiation. Journal of Applied Physics, 2014, 115, . | 1.1 | 10 |
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| 139 | Diffusion and transformation kinetics of small helium clusters in bulk tungsten. Physical Review B, 2014, 90, . | 1.1 | 79 |
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