# Jincheng Du

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9482036/publications.pdf

Version: 2024-02-01

| 175 | 5,940 | 71102 | 106344 |
|---|---|---|---|
| papers | citations | 41 h-index | 65 g-index |

| 189 | 189 | 189 | 4667 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Molecular Dynamics Simulation of the Structure and Hydroxylation of Silica Glass Surfaces. Journal of the American Ceramic Society, 2005, 88, 2532-2539. | 3.8 | 165 |
| 2 | Title is missing!. Journal of Sol-Gel Science and Technology, 2000, 17, 163-171. | 2.4 | 154 |
| 3 | Three-dimensional structure determination from a single view. Nature, 2010, 463, 214-217. | 27.8 | 153 |
| 4 | A comparative review of the aqueous corrosion of glasses, crystalline ceramics, and metals. Npj Materials Degradation, 2018, 2, . | 5.8 | 150 |
| 5 | Effect of Strontium Substitution on the Structure of 45S5 Bioglasses. Chemistry of Materials, 2011, 23, 2703-2717. | 6.7 | 135 |
| 6 | Molecular dynamics simulations of sodaâ€“limeâ€“silicate glasses. Journal of Non-Crystalline Solids, 2001, 293-295, 283-289. | 3.1 | 133 |
| 7 | Bioactive glass coatings on metallic implants for biomedical applications. Bioactive Materials, 2019, 4, 261-270. | 15.6 | 130 |
| 8 | Compositional dependence of the first sharp diffraction peaks in alkali silicate glasses: A molecular dynamics study. Journal of Non-Crystalline Solids, 2006, 352, 3255-3269. | 3.1 | 128 |
| 9 | Structure and properties of sodium aluminosilicate glasses from molecular dynamics simulations. Journal of Chemical Physics, 2013, 139, 044507. | 3.0 | 127 |
| 10 | Development of boron oxide potentials for computer simulations of multicomponent oxide glasses. Journal of the American Ceramic Society, 2019, 102, 2482-2505. | 3.8 | 124 |
| 11 | Water Interactions with Nanoporous Silica: Comparison of ReaxFF and ab Initio based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 24803-24816. | 3.1 | 94 |
| 12 | Phaseâ€Selective Nanocrystallization of NaLnF<sub>4</sub> in Aluminosilicate Glass for Random Laser and 940 nm LEDâ€Excitable Upconverted Luminescence. Laser and Photonics Reviews, 2018, 12, 1800030. | 8.7 | 94 |
| 13 | Dynamics of self-reorganization explains passivation of silicate glasses. Nature Communications, 2018, 9, 2169. | 12.8 | 94 |
| 14 | Structure of International Simple Glass and properties of passivating layer formed in circumneutral pH conditions. Npj Materials Degradation, 2018, 2, . | 5.8 | 91 |
| 15 | Molecular Dynamics Simulations of the Structure and Properties of Low Silica Yttrium Aluminosilicate Glasses. Journal of the American Ceramic Society, 2009, 92, 87-95. | 3.8 | 86 |
| 16 | Effect of strontium substitution on the structure, ionic diffusion and dynamic properties of 45S5 Bioactive glasses. Journal of Non-Crystalline Solids, 2012, 358, 1059-1071. | 3.1 | 85 |
| 17 | Structure of Cerium Phosphate Glasses: Molecular Dynamics Simulation. Journal of the American Ceramic Society, 2011, 94, 2393-2401. | 3.8 | 84 |
| 18 | Development of effective empirical potentials for molecular dynamics simulations of the structures and properties of boroaluminosilicate glasses. Journal of Non-Crystalline Solids, 2016, 453, 177-194. | 3.1 | 82 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | First sharp diffraction peak in silicate glasses: Structure and scattering length dependence. Physical Review B, 2005, 72, . | 3.2 | 76 |
| 20 | Effects of system size and cooling rate on the structure and properties of sodium borosilicate glasses from molecular dynamics simulations. Journal of Chemical Physics, 2018, 148, 024504. | 3.0 | 75 |
| 21 | A molecular dynamics simulation interpretation of neutron and x-ray diffraction measurements on single phase Y<sub>2</sub>O<sub>3</sub>â€“Al<sub>2</sub>O<sub>3</sub>glasses. Journal of Physics Condensed Matter, 2009, 21, 205102. | 1.8 | 74 |
| 22 | Structure, dynamics, and electronic properties of lithium disilicate melt and glass. Journal of Chemical Physics, 2006, 125, 114702. | 3.0 | 73 |
| 23 | <sup>87</sup>Sr Solid-State NMR as a Structurally Sensitive Tool for the Investigation of Materials: Antiosteoporotic Pharmaceuticals and Bioactive Glasses. Journal of the American Chemical Society, 2012, 134, 12611-12628. | 13.7 | 68 |
| 24 | Lithium Ion Diffusion Mechanism in Lithium Lanthanum Titanate Solidâ€State Electrolytes from Atomistic Simulations. Journal of the American Ceramic Society, 2015, 98, 534-542. | 3.8 | 66 |
| 25 | Hydrogen bonding interactions of H2O and SiOH on a boroaluminosilicate glass corroded in aqueous solution. Npj Materials Degradation, 2020, 4, . | 5.8 | 64 |
| 26 | From Phase Separation to Nanocrystallization in Fluorosilicate Glasses: Structural Design of Highly Luminescent Glass-Ceramics. Journal of Physical Chemistry C, 2016, 120, 17726-17732. | 3.1 | 63 |
| 27 | Development of a ReaxFF Reactive Force Field for NaSiO<sub>x</sub>/Water Systems and Its Application to Sodium and Proton Self-Diffusion. Journal of Physical Chemistry C, 2018, 122, 19613-19624. | 3.1 | 63 |
| 28 | The structure of erbium doped sodium silicate glasses. Journal of Non-Crystalline Solids, 2005, 351, 2263-2276. | 3.1 | 61 |
| 29 | Self-accelerated corrosion of nuclear waste forms at material interfaces. Nature Materials, 2020, 19, 310-316. | 27.5 | 61 |
| 30 | Glass-ceramic phosphors for solid state lighting: A review. Ceramics International, 2021, 47, 2963-2980. | 4.8 | 59 |
| 31 | Workfunction tuning of zinc oxide films by argon sputtering and oxygen plasma: an experimental and computational study. Journal Physics D: Applied Physics, 2012, 45, 065301. | 2.8 | 57 |
| 32 | Characterization of the Structural and Electronic Properties of Crystalline Lithium Silicates. Journal of Physical Chemistry B, 2006, 110, 22346-22352. | 2.6 | 56 |
| 33 | Rare earth ion clustering behavior in europium doped silicate glasses: Simulation size and glass structure effect. Journal of Non-Crystalline Solids, 2012, 358, 3408-3417. | 3.1 | 52 |
| 34 | Recent Advances in Corrosion Science Applicable To Disposal of High-Level Nuclear Waste. Chemical Reviews, 2021, 121, 12327-12383. | 47.7 | 52 |
| 35 | Atomistic computer simulations of water interactions and dissolution of inorganic glasses. Npj Materials Degradation, 2017, 1, . | 5.8 | 51 |
| 36 | Effect of ZrO2 on the structure and properties of soda-lime silicate glasses from molecular dynamics simulations. Journal of Non-Crystalline Solids, 2018, 491, 141-150. | 3.1 | 51 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Interfacial Structure and Evolution of the Waterâ€“Silica Gel System by Reactive Force-Field-Based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2017, 121, 11534-11543. | 3.1 | 50 |
| 38 | Composition â€“ structure â€“ property relationships in alkali aluminosilicate glasses: A combined experimental â€“ computational approach towards designing functional glasses. Journal of Non-Crystalline Solids, 2019, 505, 144-153. | 3.1 | 48 |
| 39 | Challenges in Molecular Dynamics Simulations of Multicomponent Oxide Glasses. Springer Series in Materials Science, 2015, , 157-180. | 0.6 | 47 |
| 40 | B<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> substitution effect on structure and properties of Na<sub>2</sub>Oâ€“CaOâ€“SrOâ€“P<sub>2</sub>O<sub>5</sub>â€“SiO<sub>2</sub> bioactive glasses from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 14090-14104. | 2.8 | 47 |
| 41 | Molecular Dynamics Simulations of Water Structure and Diffusion in a 1 nm Diameter Silica Nanopore as a Function of Surface Charge and Alkali Metal Counterion Identity. Journal of Physical Chemistry C, 2018, 122, 17764-17776. | 3.1 | 47 |
| 42 | Bulk, surface structures and properties of sodium borosilicate and boroaluminosilicate nuclear waste glasses from molecular dynamics simulations. Journal of Non-Crystalline Solids, 2017, 476, 87-94. | 3.1 | 44 |
| 43 | Fundamental mechanisms of oxygen plasma-induced damage of ultralow-k organosilicate materials: The role of thermal P3 atomic oxygen. Applied Physics Letters, 2009, 94, 204102. | 3.3 | 43 |
| 44 | Understanding the structural drivers governing glassâ€“water interactions in borosilicate based model bioactive glasses. Acta Biomaterialia, 2018, 65, 436-449. | 8.3 | 43 |
| 45 | Searching for correlations between vibrational spectral features and structural parameters of silicate glass network. Journal of the American Ceramic Society, 2020, 103, 3575-3589. | 3.8 | 43 |
| 46 | Measurements of liquid and glass structures using aerodynamic levitation and in-situ high energy x-ray and neutron scattering. Journal of Non-Crystalline Solids, 2014, 383, 49-51. | 3.1 | 41 |
| 47 | Structural role of ZrO2 and its impact on properties of boroaluminosilicate nuclear waste glasses. Npj Materials Degradation, 2018, 2, . | 5.8 | 41 |
| 48 | Effect of solution condition on hydroxyapatite formation in evaluating bioactivity of B2O3 containing 45S5 bioactive glasses. Bioactive Materials, 2019, 4, 207-214. | 15.6 | 41 |
| 49 | Quantitative Structureâ€“Property Relationship (QSPR) Analysis of ZrO<sub>2</sub>-Containing Soda-Lime Borosilicate Glasses. Journal of Physical Chemistry B, 2019, 123, 1412-1422. | 2.6 | 41 |
| 50 | Structural and Mechanical Properties of Nanoporous Silica. Journal of the American Ceramic Society, 2014, 97, 772-781. | 3.8 | 40 |
| 51 | Effects of boron oxide substitution on the structure and bioactivity of SrO-containing bioactive glasses. Journal of Materials Science, 2017, 52, 8793-8811. | 3.7 | 40 |
| 52 | Physical and optical properties of the International Simple Glass. Npj Materials Degradation, 2019, 3, . | 5.8 | 37 |
| 53 | Understanding lanthanum aluminate glass structure by correlating molecular dynamics simulation results with neutron and X-ray scattering data. Journal of Non-Crystalline Solids, 2007, 353, 210-214. | 3.1 | 36 |
| 54 | First-Principles-Based Kinetic Monte Carlo Simulation of Nitric Oxide Reduction over Platinum Nanoparticles under Lean-Burn Conditions. Industrial & Engineering Chemistry Research, 2010, 49, 10364-10373. | 3.7 | 36 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Evaluating Water Reactivity at Silica Surfaces Using Reactive Potentials. Journal of Physical Chemistry C, 2018, 122, 9875-9885. | 3.1 | 35 |
| 56 | Ab initio Molecular Dynamics Simulations of the Hydroxylation of Nanoporous Silica. Journal of the American Ceramic Society, 2015, 98, 3748-3757. | 3.8 | 34 |
| 57 | Understanding the compositionâ€“structureâ€“bioactivity relationships in diopside (CaOÂ·MgOÂ·2SiO2)â€“tricalcium phosphate (3CaOÂ·P2O5) glass system. Acta Biomaterialia, 2015, 15, 210-226. | 8.3 | 34 |
| 58 | Mixed Network Former Effect on Structure, Physical Properties, and Bioactivity of 45S5 Bioactive Glasses: An Integrated Experimental and Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2018, 122, 2564-2577. | 2.6 | 34 |
| 59 | Nanoporous silica gel structures and evolution from reactive force field-based molecular dynamics simulations. Npj Materials Degradation, 2018, 2, . | 5.8 | 34 |
| 60 | Assessment of interatomic parameters for the reproduction of borosilicate glass structures via DFTâ€GIPAW calculations. Journal of the American Ceramic Society, 2019, 102, 7225-7243. | 3.8 | 34 |
| 61 | Structural Origin of the Thermal and Diffusion Behaviors of Lithium Aluminosilicate Crystal Polymorphs and Glasses. Journal of the American Ceramic Society, 2016, 99, 2823-2833. | 3.8 | 33 |
| 62 | Structural features of ISG borosilicate nuclear waste glasses revealed from high-energy X-ray diffraction and molecular dynamics simulations. Journal of Nuclear Materials, 2019, 515, 284-293. | 2.7 | 33 |
| 63 | Local Structure of Cerium in Aluminophosphate and Silicophosphate Glasses. Journal of the American Ceramic Society, 2011, 94, 2442-2451. | 3.8 | 31 |
| 64 | Composite reinforcement: Recent development of continuous glass fibers. International Journal of Applied Glass Science, 2017, 8, 23-36. | 2.0 | 31 |
| 65 | The structural and electronic properties of reduced amorphous titania. Physical Chemistry Chemical Physics, 2017, 19, 18671-18684. | 2.8 | 31 |
| 66 | Enhanced single-mode fiber laser emission by nano-crystallization of oxyfluoride glass-ceramic cores. Journal of Materials Chemistry C, 2019, 7, 5155-5162. | 5.5 | 31 |
| 67 | Molecular dynamics simulations of nanoporous organosilicate glasses using Reactive Force Field (ReaxFF). Journal of Non-Crystalline Solids, 2016, 431, 103-111. | 3.1 | 30 |
| 68 | Lithium Ion Diffusion Mechanism and Associated Defect Behaviors in Crystalline Li1+xAlxGe2â€“x(PO4)3 Solid-State Electrolytes. Journal of Physical Chemistry C, 2019, 123, 27385-27398. | 3.1 | 30 |
| 69 | Short- and medium-range structure of amorphous zircon from molecular dynamics simulations. Physical Review B, 2006, 74, . | 3.2 | 29 |
| 70 | Europium environment and clustering in europium doped silica and sodium silicate glasses. Journal of Non-Crystalline Solids, 2011, 357, 2235-2240. | 3.1 | 29 |
| 71 | Eu2+ promoted formation of molecule-like Ag and enhanced white luminescence of Ag/Eu-codoped oxyfluoride glasses. Journal of Non-Crystalline Solids, 2016, 432, 348-353. | 3.1 | 29 |
| 72 | Quantitative structure-property relationship (QSPR) analysis of calcium aluminosilicate glasses based on molecular dynamics simulations. Journal of Non-Crystalline Solids, 2020, 530, 119772. | 3.1 | 29 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Tomographic mapping of the nanoscale water-filled pore structure in corroded borosilicate glass. Npj Materials Degradation, 2020, 4, . | 5.8 | 29 |
| 74 | Effects of Al:Si and (AlÂ+ÂNa):Si ratios on the properties of the international simple glass, part II: Structure. Journal of the American Ceramic Society, 2021, 104, 183-207. | 3.8 | 29 |
| 75 | Structure and diffusion of ZnOâ€“SrOâ€“CaOâ€“Na2Oâ€“SiO2 bioactive glasses: a combined high energy X-ray diffraction and molecular dynamics simulations study. RSC Advances, 2013, 3, 5966. | 3.6 | 28 |
| 76 | A structure model for phase separated fluoroaluminosilicate glass system by molecular dynamic simulations. Journal of the European Ceramic Society, 2019, 39, 5018-5029. | 5.7 | 28 |
| 77 | Surface structures of sodium borosilicate glasses from molecular dynamics simulations. Journal of the American Ceramic Society, 2017, 100, 2516-2524. | 3.8 | 27 |
| 78 | Development of Water Reactive Potentials for Sodium Silicate Glasses. Journal of Physical Chemistry B, 2019, 123, 4452-4461. | 2.6 | 27 |
| 79 | Effects of surface initial condition on aqueous corrosion of glassâ€”A study with a model nuclear waste glass. Journal of the American Ceramic Society, 2019, 102, 1652-1664. | 3.8 | 26 |
| 80 | Reaction Mechanisms and Interfacial Behaviors of Sodium Silicate Glass in an Aqueous Environment from Reactive Force Field-Based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2019, 123, 21538-21547. | 3.1 | 26 |
| 81 | Laser coating of bioactive glasses on bioimplant titanium alloys. International Journal of Applied Glass Science, 2019, 10, 307-320. | 2.0 | 26 |
| 82 | Insights into the mechanisms controlling the residual corrosion rate of borosilicate glasses. Npj Materials Degradation, 2020, 4, . | 5.8 | 26 |
| 83 | Can a simple topological-constraints-based model predict the initial dissolution rate of borosilicate and aluminosilicate glasses?. Npj Materials Degradation, 2020, 4, . | 5.8 | 26 |
| 84 | Predicting boron coordination in multicomponent borate and borosilicate glasses using analytical models and machine learning. Journal of Non-Crystalline Solids, 2021, 553, 120490. | 3.1 | 26 |
| 85 | Templated Growth of Hexagonal Nickel Carbide Nanocrystals on Vertically Aligned Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 10424-10429. | 3.1 | 24 |
| 86 | Short- and medium-range structures of cerium aluminophosphate glasses: A molecular dynamics study. Journal of Non-Crystalline Solids, 2014, 403, 67-79. | 3.1 | 24 |
| 87 | Stabilization of Fluorescent [Ag<sub>m</sub>]<sup>n+</sup> Quantum Clusters in Multiphase Inorganic Glass-Ceramics for White LEDs. ACS Applied Nano Materials, 2019, 2, 2854-2863. | 5.0 | 24 |
| 88 | Ionic self-diffusion of Na2Oâ€“Al2O3â€“SiO2 glasses from molecular dynamics simulations. Journal of Non-Crystalline Solids, 2020, 527, 119734. | 3.1 | 24 |
| 89 | First-principles calculations of the electronic structure, phase transition and properties of ZrSiO4 polymorphs. Computational and Theoretical Chemistry, 2012, 987, 62-70. | 2.5 | 23 |
| 90 | Structural features of sodium silicate glasses from reactive force fieldâ€based molecular dynamics simulations. Journal of the American Ceramic Society, 2020, 103, 1600-1614. | 3.8 | 23 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Lithium vanado-phosphate glasses: Structure and dynamics properties studied by molecular dynamics simulations. Journal of Non-Crystalline Solids, 2014, 403, 53-61. | 3.1 | 22 |
| 92 | Investigating the structureâ€“diffusionâ€“bioactivity relationship of strontium containing bioactive glasses using molecular dynamics based computer simulations. Journal of Non-Crystalline Solids, 2016, 432, 35-40. | 3.1 | 22 |
| 93 | Stabilization of ultra-small [Ag<sub>2</sub>]<sup>2+</sup> and [Ag<sub>m</sub>]<sup>n+</sup> nano-clusters through negatively charged tetrahedrons in oxyfluoride glass networks: To largely enhance the luminescence quantum yields. Physical Chemistry Chemical Physics, 2017, 19, 22638-22645. | 2.8 | 22 |
| 94 | Pushing the limits of sensitivity and resolution for natural abundance <sup>43</sup>Ca NMR using ultra-high magnetic field (35.2 T). Chemical Communications, 2018, 54, 9591-9594. | 4.1 | 22 |
| 95 | Structural Origins of RF<sub>3</sub>/NaRF<sub>4</sub> Nanocrystal Precipitation from Phase-Separated SiO<sub>2</sub>â€“Al<sub>2</sub>O<sub>3</sub>â€“RF<sub>3</sub>â€“NaF Glasses: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2019, 123, 3024-3032. | 2.6 | 22 |
| 96 | Lanthanide doped fluorosilicate glass-ceramics: A review on experimental and theoretical progresses. Journal of Rare Earths, 2022, 40, 169-192. | 4.8 | 22 |
| 97 | Hydration and reaction mechanisms on sodium silicate glass surfaces from molecular dynamics simulations with reactive force fields. Journal of the American Ceramic Society, 2020, 103, 3676-3690. | 3.8 | 21 |
| 98 | A comparative study of the effectiveness of empirical potentials for molecular dynamics simulations of borosilicate glasses. Journal of Non-Crystalline Solids, 2021, 553, 120413. | 3.1 | 21 |
| 99 | Characterization of Ion Distributions Near the Surface of Sodium-Containing and Sodium-Depleted Calcium Aluminosilicate Melts. Journal of the American Ceramic Society, 2006, 89, 36-41. | 3.8 | 20 |
| 100 | Effect of vanadium oxide addition on thermomechanical behaviors of borosilicate glasses: Toward development of high crack resistant glasses for nuclear waste disposal. Journal of Non-Crystalline Solids, 2019, 515, 88-97. | 3.1 | 20 |
| 101 | Structure and lithium ion diffusion in lithium silicate glasses and at their interfaces with lithium lanthanum titanate crystals. Journal of Non-Crystalline Solids, 2012, 358, 3531-3538. | 3.1 | 19 |
| 102 | Semiconductor to metal transition in degenerate ZnO: Al films and the impact on its carrier scattering mechanisms and bandgap for OLED applications. Journal of Materials Science: Materials in Electronics, 2014, 25, 1492-1498. | 2.2 | 19 |
| 103 | Effects of optical dopants and laser wavelength on atom probe tomography analyses of borosilicate glasses. Journal of the American Ceramic Society, 2017, 100, 4801-4815. | 3.8 | 18 |
| 104 | Monte Carlo simulation of borosilicate glass dissolution using molecular dynamics-generated glass structures. Journal of Non-Crystalline Solids, 2019, 522, 119601. | 3.1 | 18 |
| 105 | Predicting the dissolution rate of borosilicate glasses using QSPR analysis based on molecular dynamics simulations. Journal of the American Ceramic Society, 2021, 104, 4445-4458. | 3.8 | 18 |
| 106 | Towards three-dimensional structural determination of amorphous materials at atomic resolution. Physical Review B, 2013, 88, . | 3.2 | 17 |
| 107 | Atomic and microâ€structure features of nanoporous aluminosilicate glasses from reactive molecular dynamics simulations. Journal of the American Ceramic Society, 2021, 104, 229-242. | 3.8 | 17 |
| 108 | Modeling the Structure and Dynamics of Lithium Borosilicate Glasses with Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2021, 125, 8080-8089. | 3.1 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Non-bridging oxygen dependent redox and spectroscopic properties of Cu species in phosphosilicate glasses. Journal of Alloys and Compounds, 2016, 664, 331-337. | 5.5 | 16 |
| 110 | Ion-exchange mechanisms and interfacial reaction kinetics during aqueous corrosion of sodium silicate glasses. Npj Materials Degradation, 2021, 5, . | 5.8 | 16 |
| 111 | Novel alloy polymers formed fromortho-carborane and benzene or pyridine. Journal of Physics Condensed Matter, 2013, 25, 105801. | 1.8 | 15 |
| 112 | Influence of low concentration V and Co oxide doping on the dissolution behaviors of simplified nuclear waste glasses. Journal of Non-Crystalline Solids, 2016, 452, 161-168. | 3.1 | 15 |
| 113 | A modified random network model for P<sub>2</sub>O<sub>5</sub>â€“Na<sub>2</sub>Oâ€“Al<sub>2</sub>O<sub>3</sub>â€“SiO<sub>2</sub> glass studied by molecular dynamics simulations. RSC Advances, 2021, 11, 7025-7036. | 3.6 | 15 |
| 114 | The Transformation from Translucent into Transparent Rare Earth Ions Doped Oxyfluoride Glassâ€Ceramics with Enhanced Luminescence. Advanced Optical Materials, 2022, 10, . | 7.3 | 15 |
| 115 | Mechanisms of oxygen plasma damage of amine and methyl terminated organosilicate low-k dielectrics from ab initio molecular dynamics simulations. Journal Physics D: Applied Physics, 2014, 47, 335204. | 2.8 | 14 |
| 116 | Thermal conductivity of vitreous silica from molecular dynamics simulations: The effects of force field, heat flux and system size. Journal of Chemical Physics, 2017, 146, 054504. | 3.0 | 14 |
| 117 | Ca<sup>2+</sup>/Sr<sup>2+</sup>/Ba<sup>2+</sup> dependent phase separation, nanocrystallization and photoluminescence in fluoroaluminosilicate glass. Journal of the American Ceramic Society, 2020, 103, 5796-5807. | 3.8 | 14 |
| 118 | Molecular Dynamics Simulations of Oxide Glasses. Springer Handbooks, 2019, , 1131-1155. | 0.6 | 12 |
| 119 | A critical evaluation of barium silicate glass network polymerization. Journal of Non-Crystalline Solids, 2022, 583, 121477. | 3.1 | 12 |
| 120 | Electronic structure and interfacial properties of Ge nanoclusters embedded in amorphous silica. Journal of Non-Crystalline Solids, 2010, 356, 2448-2453. | 3.1 | 11 |
| 121 | Defect structure and chemical bonding of p-type ZnO:Sb thin films prepared by pulsed laser deposition. Semiconductor Science and Technology, 2014, 29, 115019. | 2.0 | 11 |
| 122 | The influence of MoOx gap states on hole injection from aluminum doped zinc oxide with nanoscale MoOx surface layer anodes for organic light emitting diodes. Journal of Applied Physics, 2015, 118, . | 2.5 | 11 |
| 123 | Local ordering and interfacial structure between spinel crystal and aluminosilicate glasses from molecular dynamics simulations. International Journal of Applied Glass Science, 2019, 10, 41-56. | 2.0 | 11 |
| 124 | Investigation of the structural environment and chemical bonding of fluorine in Yb-doped fluorosilicate glass optical fibres. Journal of Chemical Thermodynamics, 2019, 128, 119-126. | 2.0 | 11 |
| 125 | Interfacial structures of spinel crystals with borosilicate nuclear waste glasses from molecular dynamics simulations. Journal of the American Ceramic Society, 2019, 102, 4583-4601. | 3.8 | 11 |
| 126 | Experimental characterizations and molecular dynamics simulations of the structures of lead aluminosilicate glasses. Journal of Non-Crystalline Solids, 2022, 576, 121252. | 3.1 | 11 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Reaction mechanisms of thermal atomic oxygen interaction with organosilicate low k dielectric materials from ab initio molecular dynamics simulations. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2011, 29, . | 2.1 | 10 |
| 128 | Achieving long time scale simulations of glass-forming systems. Computational and Theoretical Chemistry, 2012, 987, 122-133. | 2.5 | 10 |
| 129 | Mechanisms of AZO workfunction tuning for anode use in OLEDs: Surface dipole manipulation with plasma treatments versus nanoscale WOx and VOx interfacial layers. Journal of Applied Physics, 2017, 121, . | 2.5 | 10 |
| 130 | Structural stability, electronic and thermodynamic properties of VOPO4 polymorphs from DFT+U calculations. Computational Materials Science, 2017, 126, 326-335. | 3.0 | 10 |
| 131 | Interface structures of ZnO/MoO3 and their effect on workfunction of ZnO surfaces from first principles calculations. Computational Materials Science, 2018, 141, 162-169. | 3.0 | 10 |
| 132 | In situ pair distribution function analysis of crystallizing Fe-silicate melts. Journal of Materials Science, 2021, 56, 5637-5657. | 3.7 | 10 |
| 133 | Experimental and computational studies on stacking faults in zinc titanate. Applied Physics Letters, 2014, 104, 241903. | 3.3 | 9 |
| 134 | Spectroscopic properties of Eu-doped oxynitride glassâ€“ceramics for white light LEDs. Journal of Non-Crystalline Solids, 2014, 406, 119-126. | 3.1 | 9 |
| 135 | Effect of surface adsorption and non-stoichiometry on the workfunction of ZnO surfaces: A first principles study. Journal of Applied Physics, 2015, 117, 165304. | 2.5 | 9 |
| 136 | Surface reactions and structural evolution of organosilicate glass under Ar plasma bombardment. Computational Materials Science, 2015, 110, 287-294. | 3.0 | 9 |
| 137 | UV-induced modification of fused silica: Insights from ReaxFF-based molecular dynamics simulations. AIP Advances, 2016, 6, 095312. | 1.3 | 9 |
| 138 | Structural features and rare earth ion clustering behavior in lanthanum phosphate and aluminophosphate glasses from molecular dynamics simulations. Journal of Non-Crystalline Solids, 2022, 578, 121330. | 3.1 | 9 |
| 139 | Composition Dependence of the Atomic Structures and Properties of Sodium Aluminosilicate Glasses: Molecular Dynamics Simulations with Reactive and Nonreactive Potentials. Journal of Physical Chemistry B, 2022, 126, 5326-5342. | 2.6 | 9 |
| 140 | Effect of modifier cation field strength on the structures of magnesium oxide containing aluminoborosilicate glasses. International Journal of Applied Glass Science, 2022, 13, 554-567. | 2.0 | 9 |
| 141 | Molecular Dynamics Simulation of the Structure and Hydroxylation of Silica Glass Surfaces. Journal of the American Ceramic Society, 2005, 88, 2978-2978. | 3.8 | 8 |
| 142 | Vanadium Oxidation States and Structural Role in Aluminoborosilicate Glasses: An Integrated Experimental and Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2021, 125, 12365-12377. | 2.6 | 8 |
| 143 | Effect of boron oxide on mechanical and thermal properties of bioactive glass coatings for biomedical applications. Journal of the American Ceramic Society, 2022, 105, 3986-4008. | 3.8 | 8 |
| 144 | Reply to: How much does corrosion of nuclear waste matrices matter. Nature Materials, 2020, 19, 962-963. | 27.5 | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 145 | Temperature dependent molecular fluorescence of [Agm]n+ quantum clusters stabilized by phosphate glass networks. Physical Chemistry Chemical Physics, 2020, 22, 21307-21316. | 2.8 | 7 |
| 146 | Thermal transport properties enhancement of paraffin via encapsulation into boron nitride nanotube: a molecular dynamics study. MRS Communications, 2020, 10, 475-481. | 1.8 | 7 |
| 147 | Structures of Vanadium-Containing Silicate and Borosilicate Glasses: Vanadium Potential Development and MD Simulations. Journal of Non-Crystalline Solids, 2022, 575, 121223. | 3.1 | 7 |
| 148 | Development of a force field for modeling lithium borosilicate glasses. International Journal of Applied Glass Science, 2022, 13, 444-456. | 2.0 | 7 |
| 149 | Influence of interatomic potential and simulation procedures on the structures and properties of sodium aluminosilicate glasses from molecular dynamics simulations. Journal of Non-Crystalline Solids, 2022, 588, 121639. | 3.1 | 7 |
| 150 | Structure study of rare earth doped vitreous silica by molecular dynamics simulation. Radiation Effects and Defects in Solids, 2002, 157, 789-794. | 1.2 | 6 |
| 151 | First-principles study on the adsorption and dissociation of H2 molecules on Be(0 0 0 1) surfaces. Computational Materials Science, 2016, 117, 251-258. | 3.0 | 6 |
| 152 | Simplifying a solution to a complex puzzle. Npj Materials Degradation, 2018, 2, . | 5.8 | 6 |
| 153 | Crystallization behavior of Li1+xAlxGe2-x(PO4)3 glass-ceramics: Effect of composition and thermal treatment. Journal of Non-Crystalline Solids, 2019, 525, 119680. | 3.1 | 6 |
| 154 | Borosilicate Glasses. , 2021, , 519-539. | | 6 |
| 155 | Ab initio study of structural and mechanical property of solid molecular hydrogens. European Physical Journal B, 2015, 88, 1. | 1.5 | 5 |
| 156 | Chemical bonding in carborane/aromatic co-polymers: a first-principles analysis of experimental photoemission spectra. Molecular Simulation, 2016, 42, 39-46. | 2.0 | 5 |
| 157 | Short and medium range structures of 80GeSe<sub>2</sub>â€“20Ga<sub>2</sub>Se<sub>3</sub>chalcogenide glasses. Journal of Physics Condensed Matter, 2018, 30, 185403. | 1.8 | 5 |
| 158 | Structural Origins of BaF 2 /Ba 1 â^' x R x F 2 + x /RF 3 Nanocrystals Formation from Phase Separated Fluoroaluminosilicate Glass: A Molecular Dynamic Simulation Study. Advanced Theory and Simulations, 2019, 2, 1900062. | 2.8 | 5 |
| 159 | Atomistic Understanding of Ion Exchange Strengthening of Boroaluminosilicate Glasses: Insights from Molecular Dynamics Simulations and QSPR Analysis. Journal of Physical Chemistry B, 2022, 126, 2060-2072. | 2.6 | 5 |
| 160 | Origin of thermally induced second harmonic generation in PbOâ€“B_2O_3 glasses. Optics Letters, 2012, 37, 860. | 3.3 | 4 |
| 161 | Electro-optical performance of molybdenum oxide modified aluminum doped zinc oxide anodes in organic light emitting diodes: A comparison to indium tin oxide. Materials Express, 2016, 6, 289-294. | 0.5 | 4 |
| 162 | Structures of fluoride containing aluminosilicate low activity nuclear waste glasses: A molecular dynamics simulations study. Journal of Non-Crystalline Solids, 2020, 550, 120379. | 3.1 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 163 | Influence of O(<sup>3</sup>P)/O<sub>2</sub> Flux on the Atomic Layer Deposition of B<sub>2</sub>O<sub>3</sub> Using Trimethyl Borate at Room Temperature. Journal of Physical Chemistry C, 2020, 124, 25846-25858. | 3.1 | 4 |
| 164 | Surface Micron-Structure Engineering of Halide Perovskite Doped Glass-Ceramic and Its Ionic Transport Application. ACS Applied Energy Materials, 2022, 5, 42-51. | 5.1 | 4 |
| 165 | Elucidating the Atomic Structures of the Gel Layer Formed during Aluminoborosilicate Glass Dissolution: An Integrated Experimental and Simulation Study. Journal of Physical Chemistry C, 2022, 126, 7999-8015. | 3.1 | 4 |
| 166 | Development of potentials for molecular dynamics simulations of dry and hydrated calcium aluminosilicate glasses by force matching and refinement. Journal of Non-Crystalline Solids, 2022, 592, 121746. | 3.1 | 4 |
| 167 | Local structure, composition, and crystallization mechanism of a model two-phase â€œcomposite nanoglassâ€• Journal of Chemical Physics, 2016, 144, 064503. | 3.0 | 3 |
| 168 | Patchy particle model of hydrated amorphous silica. Journal of Non-Crystalline Solids, 2021, 556, 120555. | 3.1 | 3 |
| 169 | Second harmonic generation in N-doped Hâ€‰:â€‰SiO2 films by poling under x-ray irradiation. Journal Physics D: Applied Physics, 2013, 46, 505102. | 2.8 | 2 |
| 170 | High temperature water as a clean and etch of low-k and SiO2 films. Microelectronic Engineering, 2018, 196, 54-58. | 2.4 | 2 |
| 171 | Investigation of thermal transport properties in pillared-graphene structure using nonequilibrium molecular dynamics simulations. MRS Communications, 2020, 10, 506-511. | 1.8 | 2 |
| 172 | Ab initio study of intrinsic defects and diffusion behaviors in solid molecular hydrogens. European Physical Journal B, 2015, 88, 1. | 1.5 | 1 |
| 173 | Structure, energetics, and electronic properties of stacking fault defects in ilmenite-structured ZnTiO<sub>3</sub>. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 065015. | 2.0 | 1 |
| 174 | Investigation of thermal transport properties of copper-supported pillared-graphene structure using molecular dynamics simulations. MRS Communications, 2020, 10, 695-701. | 1.8 | 1 |
| 175 | Molecular Dynamics Simulations of Displacement Cascades in Single and Polycrystalline Zirconia. , 2009, , . | | 0 |