Ganesh Balasubramanian

List of Publications by Year in descending order

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| # | Article | lF | CITATIONS |
|----|---|------|-----------|
| 1 | Thermal conductivity of graphene with defects induced by electron beam irradiation. Nanoscale, 2016, 8, 14608-14616. | 5.6 | 187 |
| 2 | Machine learned feature identification for predicting phase and Young's modulus of low-, medium- and high-entropy alloys. Scripta Materialia, 2020, 185, 152-158. | 5.2 | 102 |
| 3 | Pyrolysis reaction networks for lignin model compounds: unraveling thermal deconstruction of β-O-4 and α-O-4 compounds. Green Chemistry, 2016, 18, 1762-1773. | 9.0 | 92 |
| 4 | Modeling of thermochemical energy storage by salt hydrates. International Journal of Heat and Mass Transfer, 2010, 53, 5700-5706. | 4.8 | 81 |
| 5 | Atomistic clustering-ordering and high-strain deformation of an Al0.1CrCoFeNi high-entropy alloy. Scientific Reports, 2016, 6, 31028. | 3.3 | 81 |
| 6 | Heat conduction across a solid-solid interface: Understanding nanoscale interfacial effects on thermal resistance. Applied Physics Letters, 2011, 99, . | 3.3 | 75 |
| 7 | Lattice distortion as an estimator of solid solution strengthening in high-entropy alloys. Materials Characterization, 2021, 172, 110877. | 4.4 | 69 |
| 8 | Dislocation dynamics in Al0.1CoCrFeNi high-entropy alloy under tensile loading. Intermetallics, 2017, 91, 31-34. | 3.9 | 59 |
| 9 | Design of high-strength refractory complex solid-solution alloys. Npj Computational Materials, 2018, 4, . | 8.7 | 56 |
| 10 | Thermal conductivity reduction through isotope substitution in nanomaterials: predictions from an analytical classical model and nonequilibrium molecular dynamics simulations. Nanoscale, 2011, 3, 3714. | 5.6 | 54 |
| 11 | An Environmentally Stable and Leadâ€Free Chalcogenide Perovskite. Advanced Functional Materials, 2020, 30, 2001387. | 14.9 | 52 |
| 12 | Effect of temperature and graphite particle fillers on thermal conductivity and viscosity of phase change material n-eicosane. International Journal of Heat and Mass Transfer, 2017, 114, 318-323. | 4.8 | 50 |
| 13 | Accelerating computational modeling and design of high-entropy alloys. Nature Computational Science, 2021, 1, 54-61. | 8.0 | 44 |
| 14 | Crystallization kinetics in AlxCrCoFeNi (0 ≤ ≤40) high-entropy alloys. Scripta Materialia, 2017, 141, 54-57. | 5.2 | 42 |
| 15 | Surface oxidation mechanism of a refractory high-entropy alloy. Npj Materials Degradation, 2019, 3, . | 5.8 | 42 |
| 16 | Impeding phonon transport through superlattices of organic–inorganic halide perovskites. RSC Advances, 2017, 7, 37015-37020. | 3.6 | 41 |
| 17 | Modifying thermal transport in electrically conducting polymers: Effects of stretching and combining polymer chains. Journal of Chemical Physics, 2012, 136, 044901. | 3.0 | 38 |
| 18 | Machine learning assisted prediction of the Young's modulus of compositionally complex alloys. Scientific Reports, 2021, 11, 17149. | 3.3 | 38 |

| # | Article | IF | CITATIONS |
|----|--|-----|-----------|
| 19 | Controlling the aqueous solubility of PNIPAM with hydrophobic molecular units. Computational Materials Science, 2017, 126, 191-203. | 3.0 | 37 |
| 20 | Unsteady nanoscale thermal transport across a solid-fluid interface. Journal of Applied Physics, 2008, 104, . | 2.5 | 36 |
| 21 | Ultralow lattice thermal conductivity of chalcogenide perovskite CaZrSe3 contributes to high thermoelectric figure of merit. Npj Computational Materials, 2019, 5, . | 8.7 | 31 |
| 22 | Superhydrophobic inkjet printed flexible graphene circuits <i>via</i> direct-pulsed laser writing. Nanoscale, 2017, 9, 19058-19065. | 5.6 | 29 |
| 23 | Predictive descriptors in machine learning and data-enabled explorations of high-entropy alloys. Computational Materials Science, 2021, 193, 110381. | 3.0 | 29 |
| 24 | Machine-learning-guided descriptor selection for predicting corrosion resistance in multi-principal element alloys. Npj Materials Degradation, 2022, 6, . | 5.8 | 29 |
| 25 | Engineering band gap and electronic transport in organic–inorganic halide perovskites by superlattices. Nanoscale, 2017, 9, 8600-8607. | 5.6 | 26 |
| 26 | Viscosity of magnetite–toluene nanofluids: Dependence on temperature and nanoparticle concentration. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 2641-2644. | 2.1 | 25 |
| 27 | Reduced Thermal Transport in the Graphene/MoS ₂ /Graphene Heterostructure: A Comparison with Freestanding Monolayers. Langmuir, 2018, 34, 3326-3335. | 3.5 | 25 |
| 28 | Solution Processing Dependent Bulk Heterojunction Nanomorphology of P3HT/PCBM Thin Films. ACS Applied Materials & Interfaces, 2019, 11, 17056-17067. | 8.0 | 25 |
| 29 | Low energy atomic traps sluggardize the diffusion in compositionally complex refractory alloys. Intermetallics, 2021, 131, 107106. | 3.9 | 25 |
| 30 | Examining the electron transport in chalcogenide perovskite BaZrS ₃ . Journal of Materials Chemistry C, 2021, 9, 3892-3900. | 5.5 | 24 |
| 31 | Vacancy formation energies and migration barriers in multi-principal element alloys. Acta Materialia, 2022, 226, 117611. | 7.9 | 24 |
| 32 | Release of stored thermochemical energy from dehydrated salts. International Journal of Heat and Mass Transfer, 2011, 54, 4856-4863. | 4.8 | 23 |
| 33 | Cuckoo searching optimal composition of multicomponent alloys by molecular simulations. Scripta Materialia, 2017, 130, 292-296. | 5.2 | 23 |
| 34 | Understanding the Extremely Poor Lattice Thermal Transport in Chalcogenide Perovskite BaZrS ₃ . ACS Applied Energy Materials, 2020, 3, 1139-1144. | 5.1 | 23 |
| 35 | Effect of Cooling Rate on the Phase Formation of AlCoCrFeNi High-Entropy Alloy. Journal of Phase Equilibria and Diffusion, 2021, 42, 772-780. | 1.4 | 23 |
| 36 | Reduced thermal conductivity of isotope substituted carbon nanomaterials: Nanotube versus graphene nanoribbon. Chemical Physics Letters, 2014, 599, 154-158. | 2.6 | 22 |

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|----|--|-----|-----------|
| 37 | Transfer Learned Designer Polymers For Organic Solar Cells. Journal of Chemical Information and Modeling, 2021, 61, 134-142. | 5.4 | 22 |
| 38 | Composition and processing dependent miscibility of P3HT and PCBM in organic solar cells by coarse-grained molecular simulations. Computational Materials Science, 2018, 155, 112-115. | 3.0 | 21 |
| 39 | Structure of aqueous MgSO4 solution: Dilute to concentrated. Chemical Physics Letters, 2011, 508, 38-42. | 2.6 | 20 |
| 40 | A Spectral Density Function Approach for Active Layer Design of Organic Photovoltaic Cells. Journal of Mechanical Design, Transactions of the ASME, 2018, 140, . | 2.9 | 20 |
| 41 | Effect of polydispersity on the bulkâ€heterojunction morphology of P3HT:PCBM solar cells. Journal of Polymer Science, Part B: Polymer Physics, 2019, 57, 895-903. | 2.1 | 20 |
| 42 | Designing anisotropic microstructures with spectral density function. Computational Materials Science, 2020, 179, 109559. | 3.0 | 20 |
| 43 | Structural and thermochemical properties of a photoresponsive spiropyran and merocyanine pair: Basis set and solvent dependence in density functional predictions. Chemical Physics Letters, 2012, 554, 60-66. | 2.6 | 19 |
| 44 | An informatics based analysis of the impact of isotope substitution on phonon modes in graphene. Applied Physics Letters, 2014, 104, . | 3.3 | 17 |
| 45 | Tuning phase stability and short-range order through Al doping in (CoCrFeMn)100â^'xAlx high-entropy alloys. Physical Review Materials, 2019, 3, . | 2.4 | 16 |
| 46 | Elastomechanical properties of resilin. Soft Matter, 2011, 7, 11006. | 2.7 | 14 |
| 47 | Shear viscosity enhancement in water–nanoparticle suspensions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 860-863. | 2.1 | 14 |
| 48 | Doping and Anisotropy–Dependent Electronic Transport in Chalcogenide Perovskite CaZrSe ₃ for High Thermoelectric Efficiency. Advanced Theory and Simulations, 2019, 2, 1900060. | 2.8 | 14 |
| 49 | Elasto-morphology of P3HT:PCBM bulk heterojunction organic solar cells. Soft Matter, 2020, 16, 6743-6751. | 2.7 | 14 |
| 50 | Grain-size effects on the deformation in nanocrystalline multi-principal element alloy. Materials Chemistry and Physics, 2022, 277, 125546. | 4.0 | 14 |
| 51 | Reducing thermal transport in electrically conducting polymers: Effects of ordered mixing of polymer chains. Applied Physics Letters, 2013, 102, 023109. | 3.3 | 13 |
| 52 | Thermal conductivity reduction in analogous 2D nanomaterials with isotope substitution: Graphene and silicene. Chemical Physics Letters, 2016, 650, 88-93. | 2.6 | 13 |
| 53 | Aptamer based electrostatic-stimuli responsive surfaces for on-demand binding/unbinding of a specific ligand. Journal of Materials Chemistry B, 2017, 5, 3675-3685. | 5.8 | 13 |
| 54 | Azobenzene switch with a long-lived cis-state to photocontrol the enzyme activity of a histone deacetylase-like amidohydrolase. Biological Chemistry, 2014, 395, 401-412. | 2.5 | 12 |

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| 55 | Electrical Stimulus Controlled Binding/Unbinding of Human Thrombin-Aptamer Complex. Scientific Reports, 2016, 6, 37449. | 3.3 | 12 |
| 56 | A novel ceramic derived processing route for Multi-Principal Element Alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2020, 793, 139892. | 5.6 | 11 |
| 57 | Pseudoelastic deformation in Mo-based refractory multi-principal element alloys. Acta Materialia, 2021, 220, 117299. | 7.9 | 11 |
| 58 | Effect of heterostructure engineering on electronic structure and transport properties of two-dimensional halide perovskites. Computational Materials Science, 2021, 200, 110823. | 3.0 | 10 |
| 59 | Influence of longitudinal isotope substitution on the thermal conductivity of carbon nanotubes: Results of nonequilibrium molecular dynamics and local density functional calculations. Journal of Chemical Physics, 2014, 140, 144704. | 3.0 | 9 |
| 60 | Investigating blend morphology of P3HT:PCBM bulk heterojunction solar cells by classical atomistic simulations – Progress and prospects. Soft Materials, 2020, 18, 163-176. | 1.7 | 9 |
| 61 | Data-Guided Feature Identification for Predicting Specific Heat of Multicomponent Alloys. Jom, 2022, 74, 1406-1413. | 1.9 | 9 |
| 62 | Examining the thermodynamic stability of mixed principal element oxides in AlCoCrFeNi high-entropy alloy by first-principles. Computational Materials Science, 2022, 213, 111619. | 3.0 | 9 |
| 63 | Dynamics of impinging nanoscale jets. Chemical Physics Letters, 2010, 491, 177-182. | 2.6 | 7 |
| 64 | Machine learned metaheuristic optimization of the bulk heterojunction morphology in P3HT:PCBM thin films. Computational Materials Science, 2021, 187, 110119. | 3.0 | 7 |
| 65 | Scalable Adaptive Batch Sampling in Simulation-Based Design With Heteroscedastic Noise. Journal of Mechanical Design, Transactions of the ASME, 2021, 143, . | 2.9 | 7 |
| 66 | Optimizing isotope substitution in graphene for thermal conductivity minimization by genetic algorithm driven molecular simulations. Applied Physics Letters, 2017, 110, 133107. | 3.3 | 6 |
| 67 | Force spectroscopy of the thrombin-aptamer interaction: Comparison between AFM experiments and molecular dynamics simulations. Applied Surface Science, 2019, 475, 462-472. | 6.1 | 6 |
| 68 | Examining oxidation in β-NiAl and β-NiAl+Hf alloys by stochastic cellular automata simulations. Npj Materials Degradațion, 2021, 5, | 5.8 | 6 |
| 69 | xmins:mmi="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"> <mmi:msub><mmi:mrow /><mmi:mn>2</mmi:mn></mmi:mrow </mmi:msub> O <mmi:math xmins:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mmi:msub><mmi:mrow /><mmi:mn>3</mmi:mn></mmi:mrow </mmi:msub> and Al<mmi:math< td=""><td>2.7</td><td>6</td></mmi:math<></mmi:math | 2.7 | 6 |
| 70 | xmlns:mml="http://www.w3.org/1998/Math/MathMt" altimg="sl1.svg"> <mml:msub><mml:mrow /><mml: A Spectral Density Function Approach for Design of Organic Photovoltaic Cells. , 2018, , .</mml: </mml:mrow </mml:msub> | | 5 |
| 71 | Energetic and structural properties of different conformations of merocyanine and its protonated forms. Chemical Physics Letters, 2015, 633, 287-291. | 2.6 | 4 |
| 72 | Transient evaporation of water thin film over nanostructured graphene. Applied Surface Science, 2019, 495, 143545. | 6.1 | 4 |

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|----|--|------|-----------|
| 73 | Effect of oxidation on the thermal expansion of a refractory multicomponent alloy. Philosophical Magazine Letters, 2021, 101, 173-182. | 1.2 | 4 |
| 74 | Directed Energy Deposition of Multi-Principal Element Alloys. Frontiers in Materials, 2022, 9, . | 2.4 | 4 |
| 75 | Designing active layer of organic solar cells using multi-fidelity molecular simulations and spectral density function. Computational Materials Science, 2022, 211, 111491. | 3.0 | 4 |
| 76 | Comparison of laser deposition methods for the synthesis of AlxCoCrFeNi multi-principal element alloy. Journal of Materials Research and Technology, 2022, 19, 1090-1101. | 5.8 | 4 |
| 77 | Predicting mode-dependent phonon thermal conductivity of silicon nanoparticle using Boltzmann transport equation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2761-2764. | 2.1 | 3 |
| 78 | Elongated Nanodomains and Molecular Intermixing Induced Doping in Organic Photovoltaic Active Layers with Electric Field Treatment. ACS Applied Polymer Materials, 2020, 2, 335-341. | 4.4 | 3 |
| 79 | Effect of vacancy defects on the thermal transport of β-Ga ₂ O ₃ . Molecular Simulation, 2021, 47, 1017-1021. | 2.0 | 3 |
| 80 | A Process Parameter Predictive Framework for Laser Cladding of Multi-principal Element Alloys. Additive Manufacturing Letters, 2022, , 100045. | 2.1 | 3 |
| 81 | Community Approaches To Recycling Plastics. , 2019, , . | | 2 |
| 82 | Neural-network model for force prediction in multi-principal-element alloys. Computational Materials Science, 2021, 198, 110693. | 3.0 | 2 |
| 83 | Towards Improving the Efficiency of Organic Solar Cells by Coarse-Grained Atomistic Modeling of Processing Dependent Morphologies. Computing in Science and Engineering, 2021, 23, 48-55. | 1.2 | 2 |
| 84 | Comparing the Properties of Polyethylene Terephthalate (PET) Plastic Bricks to Conventional Concrete Masonry Units. , 2020, , . | | 2 |
| 85 | Scalable Objective-Driven Batch Sampling in Simulation-Based Design for Models With Heteroscedastic Noise. , 2020, , . | | 2 |
| 86 | Thermochemical Energy Storage Using Salt Hydrates. , 2010, , . | | 1 |
| 87 | Effect of metallic nanoparticle fillers on the thermal conductivity of diatomaceous earth. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 3645-3649. | 2.1 | 1 |
| 88 | Understanding the anisotropic phonon thermal transport through 2D β-siligraphene. Carbon, 2021, 179, 523-530. | 10.3 | 1 |
| 89 | Tuning bandgap and energy stability of Organic-Inorganic halide perovskites through surface engineering. Computational Materials Science, 2022, 213, 111649. | 3.0 | 1 |
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90 Interfacial Thermal Resistance in Nanoscale Heat Transfer. , 2008, , .

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|----|--|-----|-----------|
| 91 | Multiscale Thermal Transport Across Solid-Solid Interfaces. , 2010, , . | | 0 |
| 92 | A Heterogeneous Multiscale Model for Interfacial Thermal Transport. , 2010, , . | | 0 |
| 93 | Pseudoelastic Deformation in Refractory (MoW) ₈₅ Zr _{7.5} (TaTi) _{7.5} High-Entropy Alloy. SSRN Electronic Journal, 0, , . | 0.4 | Ο |
| 94 | Grain-Size Effects on the Deformation in Nanocrystalline Multi-Principal Element Alloy. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 95 | Machine Learned Feature Identification for Predicting Phase and Young's Modulus of Low-, Medium- and High-Entropy Alloys. SSRN Electronic Journal, 0, , . | 0.4 | Ο |
| 96 | Direct Observations of Uniform Bulk Heterojunctions and the Energy Level Alignments in Nonfullerene Organic Photovoltaic Active Layers. ACS Applied Materials & Interfaces, 2021, 13, 56430-56437. | 8.0 | 0 |
| 97 | Examining the effect of flake orientation on the hydrophilicity of MoS2 by molecular simulations. Chemical Physics Letters, 2022, 787, 139271. | 2.6 | 0 |
| 98 | Analyzing Security Risks in Cyber-Physical Manufacturing Systems with Actor–Network Theory. Smart and Sustainable Manufacturing Systems, 2022, 6, 110-121. | 0.7 | 0 |