

# Ganesh Balasubramanian

## List of Publications by Year in descending order

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98  
papers

2,159  
citations

236612

25  
h-index

264894

42  
g-index

100  
all docs

100  
docs citations

100  
times ranked

2458  
citing authors

#	ARTICLE	IF	CITATIONS
1	Thermal conductivity of graphene with defects induced by electron beam irradiation. <i>Nanoscale</i> , 2016, 8, 14608-14616.	2.8	187
2	Machine learned feature identification for predicting phase and Young's modulus of low-, medium- and high-entropy alloys. <i>Scripta Materialia</i> , 2020, 185, 152-158.	2.6	102
3	Pyrolysis reaction networks for lignin model compounds: unraveling thermal deconstruction of ̢ <sup>2</sup> -O-4 and ̢ <sup>5</sup> -O-4 compounds. <i>Green Chemistry</i> , 2016, 18, 1762-1773.	4.6	92
4	Modeling of thermochemical energy storage by salt hydrates. <i>International Journal of Heat and Mass Transfer</i> , 2010, 53, 5700-5706.	2.5	81
5	Atomistic clustering-ordering and high-strain deformation of an Al <sub>0.1</sub> CrCoFeNi high-entropy alloy. <i>Scientific Reports</i> , 2016, 6, 31028.	1.6	81
6	Heat conduction across a solid-solid interface: Understanding nanoscale interfacial effects on thermal resistance. <i>Applied Physics Letters</i> , 2011, 99, .	1.5	75
7	Lattice distortion as an estimator of solid solution strengthening in high-entropy alloys. <i>Materials Characterization</i> , 2021, 172, 110877.	1.9	69
8	Dislocation dynamics in Al <sub>0.1</sub> CoCrFeNi high-entropy alloy under tensile loading. <i>Intermetallics</i> , 2017, 91, 31-34.	1.8	59
9	Design of high-strength refractory complex solid-solution alloys. <i>Npj Computational Materials</i> , 2018, 4, .	3.5	56
10	Thermal conductivity reduction through isotope substitution in nanomaterials: predictions from an analytical classical model and nonequilibrium molecular dynamics simulations. <i>Nanoscale</i> , 2011, 3, 3714.	2.8	54
11	An Environmentally Stable and Lead-free Chalcogenide Perovskite. <i>Advanced Functional Materials</i> , 2020, 30, 2001387.	7.8	52
12	Effect of temperature and graphite particle fillers on thermal conductivity and viscosity of phase change material n-eicosane. <i>International Journal of Heat and Mass Transfer</i> , 2017, 114, 318-323.	2.5	50
13	Accelerating computational modeling and design of high-entropy alloys. <i>Nature Computational Science</i> , 2021, 1, 54-61.	3.8	44
14	Crystallization kinetics in Al <sub>x</sub> CrCoFeNi (0 ≤ x ≤ 40) high-entropy alloys. <i>Scripta Materialia</i> , 2017, 141, 54-57.	2.6	42
15	Surface oxidation mechanism of a refractory high-entropy alloy. <i>Npj Materials Degradation</i> , 2019, 3, .	2.6	42
16	Impeding phonon transport through superlattices of organic-inorganic halide perovskites. <i>RSC Advances</i> , 2017, 7, 37015-37020.	1.7	41
17	Modifying thermal transport in electrically conducting polymers: Effects of stretching and combining polymer chains. <i>Journal of Chemical Physics</i> , 2012, 136, 044901.	1.2	38
18	Machine learning assisted prediction of the Young's modulus of compositionally complex alloys. <i>Scientific Reports</i> , 2021, 11, 17149.	1.6	38

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19	Controlling the aqueous solubility of PNIPAM with hydrophobic molecular units. Computational Materials Science, 2017, 126, 191-203.	1.4	37
20	Unsteady nanoscale thermal transport across a solid-fluid interface. Journal of Applied Physics, 2008, 104, .	1.1	36
21	Ultralow lattice thermal conductivity of chalcogenide perovskite CaZrSe <sub>3</sub> contributes to high thermoelectric figure of merit. Npj Computational Materials, 2019, 5, .	3.5	31
22	Superhydrophobic inkjet printed flexible graphene circuits <i>via</i> direct-pulsed laser writing. Nanoscale, 2017, 9, 19058-19065.	2.8	29
23	Predictive descriptors in machine learning and data-enabled explorations of high-entropy alloys. Computational Materials Science, 2021, 193, 110381.	1.4	29
24	Machine-learning-guided descriptor selection for predicting corrosion resistance in multi-principal element alloys. Npj Materials Degradation, 2022, 6, .	2.6	29
25	Engineering band gap and electronic transport in organic-inorganic halide perovskites by superlattices. Nanoscale, 2017, 9, 8600-8607.	2.8	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.	0.9	25
27	Reduced Thermal Transport in the Graphene/MoS <sub>2</sub> /Graphene Heterostructure: A Comparison with Freestanding Monolayers. Langmuir, 2018, 34, 3326-3335.	1.6	25
28	Solution Processing Dependent Bulk Heterojunction Nanomorphology of P3HT/PCBM Thin Films. ACS Applied Materials & Interfaces, 2019, 11, 17056-17067.	4.0	25
29	Low energy atomic traps sluggardize the diffusion in compositionally complex refractory alloys. Intermetallics, 2021, 131, 107106.	1.8	25
30	Examining the electron transport in chalcogenide perovskite BaZrS <sub>3</sub> . Journal of Materials Chemistry C, 2021, 9, 3892-3900.	2.7	24
31	Vacancy formation energies and migration barriers in multi-principal element alloys. Acta Materialia, 2022, 226, 117611.	3.8	24
32	Release of stored thermochemical energy from dehydrated salts. International Journal of Heat and Mass Transfer, 2011, 54, 4856-4863.	2.5	23
33	Cuckoo searching optimal composition of multicomponent alloys by molecular simulations. Scripta Materialia, 2017, 130, 292-296.	2.6	23
34	Understanding the Extremely Poor Lattice Thermal Transport in Chalcogenide Perovskite BaZrS <sub>3</sub> . ACS Applied Energy Materials, 2020, 3, 1139-1144.	2.5	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.	0.5	23
36	Reduced thermal conductivity of isotope substituted carbon nanomaterials: Nanotube versus graphene nanoribbon. Chemical Physics Letters, 2014, 599, 154-158.	1.2	22

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37	Transfer Learned Designer Polymers For Organic Solar Cells. Journal of Chemical Information and Modeling, 2021, 61, 134-142.	2.5	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.	1.4	21
39	Structure of aqueous MgSO <sub>4</sub> solution: Dilute to concentrated. Chemical Physics Letters, 2011, 508, 38-42.	1.2	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, .	1.7	20
41	Effect of polydispersity on the bulk heterojunction morphology of P3HT:PCBM solar cells. Journal of Polymer Science, Part B: Polymer Physics, 2019, 57, 895-903.	2.4	20
42	Designing anisotropic microstructures with spectral density function. Computational Materials Science, 2020, 179, 109559.	1.4	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.	1.2	19
44	An informatics based analysis of the impact of isotope substitution on phonon modes in graphene. Applied Physics Letters, 2014, 104, .	1.5	17
45	Tuning phase stability and short-range order through Al doping in (CoCrFeMn) <sub>100-x</sub> Al <sub>x</sub> high-entropy alloys. Physical Review Materials, 2019, 3, .	0.9	16
46	Elastomechanical properties of resilin. Soft Matter, 2011, 7, 11006.	1.2	14
47	Shear viscosity enhancement in water nanoparticle suspensions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 860-863.	0.9	14
48	Doping and Anisotropy Dependent Electronic Transport in Chalcogenide Perovskite CaZrSe <sub>3</sub> for High Thermoelectric Efficiency. Advanced Theory and Simulations, 2019, 2, 1900060.	1.3	14
49	Elasto-morphology of P3HT:PCBM bulk heterojunction organic solar cells. Soft Matter, 2020, 16, 6743-6751.	1.2	14
50	Grain-size effects on the deformation in nanocrystalline multi-principal element alloy. Materials Chemistry and Physics, 2022, 277, 125546.	2.0	14
51	Reducing thermal transport in electrically conducting polymers: Effects of ordered mixing of polymer chains. Applied Physics Letters, 2013, 102, 023109.	1.5	13
52	Thermal conductivity reduction in analogous 2D nanomaterials with isotope substitution: Graphene and silicene. Chemical Physics Letters, 2016, 650, 88-93.	1.2	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.	2.9	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.	1.2	12

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55	Electrical Stimulus Controlled Binding/Unbinding of Human Thrombin-Aptamer Complex. Scientific Reports, 2016, 6, 37449.	1.6	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.	2.6	11
57	Pseudoelastic deformation in Mo-based refractory multi-principal element alloys. Acta Materialia, 2021, 220, 117299.	3.8	11
58	Effect of heterostructure engineering on electronic structure and transport properties of two-dimensional halide perovskites. Computational Materials Science, 2021, 200, 110823.	1.4	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.	1.2	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.	0.8	9
61	Data-Guided Feature Identification for Predicting Specific Heat of Multicomponent Alloys. Jom, 2022, 74, 1406-1413.	0.9	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.	1.4	9
63	Dynamics of impinging nanoscale jets. Chemical Physics Letters, 2010, 491, 177-182.	1.2	7
64	Machine learned metaheuristic optimization of the bulk heterojunction morphology in P3HT:PCBM thin films. Computational Materials Science, 2021, 187, 110119.	1.4	7
65	Scalable Adaptive Batch Sampling in Simulation-Based Design With Heteroscedastic Noise. Journal of Mechanical Design, Transactions of the ASME, 2021, 143, .	1.7	7
66	Optimizing isotope substitution in graphene for thermal conductivity minimization by genetic algorithm driven molecular simulations. Applied Physics Letters, 2017, 110, 133107.	1.5	6
67	Force spectroscopy of the thrombin-aptamer interaction: Comparison between AFM experiments and molecular dynamics simulations. Applied Surface Science, 2019, 475, 462-472.	3.1	6
68	Examining oxidation in $\hat{1}^2$ -NiAl and $\hat{1}^2$ -NiAl+Hf alloys by stochastic cellular automata simulations. Npj Materials Degradation, 2021, 5, .	2.6	6
69	Examining the thermodynamic stability of mixed principal element oxides through stable Cr $\langle$ mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math> and Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>	1.3	6
70	A Spectral Density Function Approach for Design of Organic Photovoltaic Cells. , 2018, , .		5
71	Energetic and structural properties of different conformations of merocyanine and its protonated forms. Chemical Physics Letters, 2015, 633, 287-291.	1.2	4
72	Transient evaporation of water thin film over nanostructured graphene. Applied Surface Science, 2019, 495, 143545.	3.1	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.	0.5	4
74	Directed Energy Deposition of Multi-Principal Element Alloys. Frontiers in Materials, 2022, 9, .	1.2	4
75	Designing active layer of organic solar cells using multi-fidelity molecular simulations and spectral density function. Computational Materials Science, 2022, 211, 111491.	1.4	4
76	Comparison of laser deposition methods for the synthesis of Al <sub>x</sub> CoCrFeNi multi-principal element alloy. Journal of Materials Research and Technology, 2022, 19, 1090-1101.	2.6	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.	0.9	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.	2.0	3
79	Effect of vacancy defects on the thermal transport of $\hat{I}^2$ -Ga <sub>2</sub> O <sub>3</sub> . Molecular Simulation, 2021, 47, 1017-1021.	0.9	3
80	A Process Parameter Predictive Framework for Laser Cladding of Multi-principal Element Alloys. Additive Manufacturing Letters, 2022, , 100045.	0.9	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.	1.4	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.	0.9	1
88	Understanding the anisotropic phonon thermal transport through 2D $\hat{I}^2$ -siligraphene. Carbon, 2021, 179, 523-530.	5.4	1
89	Tuning bandgap and energy stability of Organic-Inorganic halide perovskites through surface engineering. Computational Materials Science, 2022, 213, 111649.	1.4	1
90	Interfacial Thermal Resistance in Nanoscale Heat Transfer. , 2008, , .		0

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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) $\langle \text{sub} \rangle 85 \langle / \text{sub} \rangle$ Zr $\langle \text{sub} \rangle 7.5 \langle / \text{sub} \rangle$ (TaTi) $\langle \text{sub} \rangle 7.5 \langle / \text{sub} \rangle$ High-Entropy Alloy. SSRN Electronic Journal, 0, , .	0.4	0
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	0
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.	4.0	0
97	Examining the effect of flake orientation on the hydrophilicity of MoS <sub>2</sub> by molecular simulations. Chemical Physics Letters, 2022, 787, 139271.	1.2	0
98	Analyzing Security Risks in Cyber-Physical Manufacturing Systems with Actor-€"Network Theory. Smart and Sustainable Manufacturing Systems, 2022, 6, 110-121.	0.3	0