Vikas Varshney

List of Publications by Year in descending order

73 papers	5,225 citations	185998 28 h-index	95083 68 g-index
74 all docs	74 docs citations	74 times ranked	7506 citing authors

#	Article	IF	Citations
1	Creep Mechanics of Epoxy Vitrimer Materials. ACS Applied Polymer Materials, 2022, 4, 4254-4263.	2.0	21
2	Machine learning strategies for the structure-property relationship of copolymers. IScience, 2022, 25, 104585.	1.9	16
3	Molecular modeling for predicting material and junction strengths of various carbon nanostructures. , 2021, , 67-102.		0
4	Molecular dynamics methodologies for predicting thermal transport in aerospace polymers and their composites. , 2021, , 19-34.		0
5	Transesterification in Vitrimer Polymers Using Bifunctional Catalysts: Modeled with Solution-Phase Experimental Rates and Theoretical Analysis of Efficiency and Mechanisms. Journal of Physical Chemistry B, 2021, 125, 2411-2424.	1.2	30
6	Vitrimer Transition Temperature Identification: Coupling Various Thermomechanical Methodologies. ACS Applied Polymer Materials, 2021, 3, 1756-1766.	2.0	47
7	A study on mechanical strength and stability of partially-fused carbon nanotube junctions. Carbon Trends, 2021, 3, 100039.	1.4	2
8	Breaking the bottleneck: stilbene as a model compound for optimizing 6Ï€ e^{âˆ’} photocyclization efficiency. RSC Advances, 2021, 11, 6504-6508.	1.7	3
9	Benchmarking Machine Learning Models for Polymer Informatics: An Example of Glass Transition Temperature. Journal of Chemical Information and Modeling, 2021, 61, 5395-5413.	2.5	59
10	Multi-Terminal Nanotube Junctions: Modeling and Structure-Property Relationship. Frontiers in Materials, 2021, 8, .	1.2	1
11	Emerging Applications of Elemental 2D Materials. Advanced Materials, 2020, 32, e1904302.	11.1	336
12	Hierarchical Assembly of Gold Nanoparticles on Graphene Nanoplatelets by Spontaneous Reduction: Implications for Smart Composites and Biosensing. ACS Applied Nano Materials, 2020, 3, 8753-8762.	2.4	13
13	Molecular dynamics simulations of separator-cathode interfacial thermal transport in a Li-ion cell. Surfaces and Interfaces, 2020, 21, 100674.	1.5	11
14	Calculation of specific heat of polymers using molecular dynamics simulations. Polymer, 2019, 167, 176-181.	1.8	20
15	Embedded optical nanosensors for monitoring the processing and performance of polymer matrix composites. Journal of Materials Chemistry C, 2019, 7, 14471-14492.	2.7	9
16	Polytypism in ultrathin tellurium. 2D Materials, 2019, 6, 015013.	2.0	68
17	Molecular Modeling of Cross-Linked Polymers with Complex Cure Pathways: A Case Study of Bismaleimide Resins. Macromolecules, 2018, 51, 1830-1840.	2.2	64
18	Computer-aided design of three terminal (3T-) zig-zag SWCNT junctions and nanotube architectures. Composites Science and Technology, 2018, 166, 36-45.	3.8	2

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19	Bond saturation significantly enhances thermal energy transport in two-dimensional pentagonal materials. Nano Energy, 2018, 45, 1-9.	8.2	15
20	Developing nanotube junctions with arbitrary specifications. Nanoscale, 2018, 10, 403-415.	2.8	7
21	Thermal Reshaping Dynamics of Gold Nanorods: Influence of Size, Shape, and Local Environment. ACS Applied Materials & Interfaces, 2018, 10, 43865-43873.	4.0	23
22	Effect of Length, Diameter, Chirality, Deformation, and Strain on Contact Thermal Conductance Between Single-Wall Carbon Nanotubes. Frontiers in Materials, 2018, 5, .	1.2	16
23	In situ mechanical investigation of carbon nanotubeâ€“graphene junction in three-dimensional carbon nanostructures. Nanoscale, 2017, 9, 2916-2924.	2.8	41
24	2D Heterostructure coatings of<i>h</i>BN-MoS₂layers for corrosion resistance. Journal Physics D: Applied Physics, 2017, 50, 045301.	1.3	19
25	How to characterize thermal transport capability of 2D materials fairly? â€“ Sheet thermal conductance and the choice of thickness. Chemical Physics Letters, 2017, 669, 233-237.	1.2	103
26	Understanding thermal conductance across multi-wall carbon nanotube contacts: Role of nanotube curvature. Carbon, 2017, 114, 15-22.	5.4	18
27	Investigation of phonon transport and thermal boundary conductance at the interface of functionalized SWCNT and poly (ether-ketone). Journal of Applied Physics, 2016, 120, .	1.1	11
28	In silico carbon molecular beam epitaxial growth of graphene on the h-BN substrate: carbon source effect on van der Waals epitaxy. Nanoscale, 2016, 8, 9704-9713.	2.8	9
29	Hydrogenation of Penta-Graphene Leads to Unexpected Large Improvement in Thermal Conductivity. Nano Letters, 2016, 16, 3925-3935.	4.5	142
30	Thermal Conductivity of Wurtzite Zinc-Oxide from First-Principles Lattice Dynamics â€“ a Comparative Study with Gallium Nitride. Scientific Reports, 2016, 6, 22504.	1.6	119
31	Multiphysics characterization of multi-walled carbon nanotube thermoplastic polyurethane polymer nanocomposites during compression. Carbon, 2016, 98, 638-648.	5.4	11
32	Nanoscale TiO2 films and their application in remediation of organic pollutants. Coordination Chemistry Reviews, 2016, 306, 43-64.	9.5	121
33	Modeling for predicting strength of carbon nanostructures. Carbon, 2015, 95, 181-189.	5.4	17
34	Modeling the Role of Bulk and Surface Characteristics of Carbon Fiber on Thermal Conductance across the Carbon-Fiber/Matrix Interface. ACS Applied Materials & Interfaces, 2015, 7, 26674-26683.	4.0	25
35	Molecular Modeling of Interfaces between Hole Transport and Active Layers in Flexible Organic Electronic Devices. Journal of Physical Chemistry C, 2015, 119, 27909-27918.	1.5	12
36	Modeling of cross-plane interface thermal conductance between graphene nano-ribbons. 2D Materials, 2014, 1, 025005.	2.0	9

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37	Thermal anisotropy in nano-crystalline MoS₂thin films. Physical Chemistry Chemical Physics, 2014, 16, 1008-1014.	1.3	63
38	Prediction of Specific Biomolecule Adsorption on Silica Surfaces as a Function of pH and Particle Size. Chemistry of Materials, 2014, 26, 5725-5734.	3.2	125
39	Force Field and a Surface Model Database for Silica to Simulate Interfacial Properties in Atomic Resolution. Chemistry of Materials, 2014, 26, 2647-2658.	3.2	369
40	Effect of Curing and Functionalization on the Interface Thermal Conductance in Carbon Nanotubeâ€“Epoxy Composites. Jom, 2013, 65, 140-146.	0.9	29
41	Scaling law for energy bandgap and effective electron mass in graphene nano mesh. Applied Physics Letters, 2013, 102, 203107.	1.5	22
42	Superior thermal interface via vertically aligned carbon nanotubes grown on graphite foils. Journal of Materials Research, 2013, 28, 933-939.	1.2	17
43	Single mode phonon scattering at carbon nanotube-graphene junction in pillared graphene structure. Applied Physics Letters, 2012, 100, 183111.	1.5	36
44	How does CNT Functionalization and Epoxy Curing affects the Thermal Interface Conductance in CNT-Epoxy Composites? An atomistic modeling perspective. , 2012, , .		0
45	Heat Transfer at Aluminumâ€“Water Interfaces: Effect of Surface Roughness. Journal of Nanotechnology in Engineering and Medicine, 2012, 3, .	0.8	8
46	Heat Transfer at Aluminum-Water Interfaces: Effect of Surface Roughness. , 2012, , .		1
47	Effects of Titanium-Containing Additives on the Dehydrogenation Properties of LiAlH₄: A Computational and Experimental Study. Journal of Physical Chemistry C, 2012, 116, 22327-22335.	1.5	18
48	A novel nano-configuration for thermoelectrics: helicity induced thermal conductivity reduction in nanowires. Nanoscale, 2012, 4, 5009.	2.8	18
49	Importance of Interfaces in Governing Thermal Transport in Composite Materials: Modeling and Experimental Perspectives. ACS Applied Materials & Interfaces, 2012, 4, 545-563.	4.0	67
50	Temperature dependence of thermal conductance between aluminum and water. International Journal of Thermal Sciences, 2012, 59, 17-20.	2.6	2
51	Thermal properties of graphene: Fundamentals and applications. MRS Bulletin, 2012, 37, 1273-1281.	1.7	1,309
52	Helicity induced thermal conductivity reduction in superlattice nanowires. , 2012, , .		0
53	Thermal Rectification in Three-Dimensional Asymmetric Nanostructure. Nano Letters, 2012, 12, 3491-3496.	4.5	66
54	Prediction of 3D elastic moduli and Poissonâ€™s ratios of pillared graphene nanostructures. Carbon, 2012, 50, 603-611.	5.4	59

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55	Modeling of interface thermal conductance in longitudinally connected carbon nanotube junctions. Journal of Applied Physics, 2011, 109, .	1.1	24
56	Preparation of Tunable 3D Pillared Carbon Nanotubeâ€"Graphene Networks for High-Performance Capacitance. Chemistry of Materials, 2011, 23, 4810-4816.	3.2	367
57	Molecular dynamics simulations of thermal transport in porous nanotube network structures. Nanoscale, 2011, 3, 3679.	2.8	31
58	Single mode phonon energy transmission in functionalized carbon nanotubes. Journal of Chemical Physics, 2011, 135, 104109.	1.2	12
59	Thermal interface tailoring in composite materials. Diamond and Related Materials, 2010, 19, 268-272.	1.8	9
60	Modeling of Thermal Conductance at Transverse CNTâ^'CNT Interfaces. Journal of Physical Chemistry C, 2010, 114, 16223-16228.	1.5	80
61	MD simulations of molybdenum disulphide (MoS2): Force-field parameterization and thermal transport behavior. Computational Materials Science, 2010, 48, 101-108.	1.4	158
62	Modeling of Mechanical Behavior of Pillard Graphene Structures. , 2010, , .		1
63	Modeling of Thermal Transport in Pillared-Graphene Architectures. ACS Nano, 2010, 4, 1153-1161.	7.3	280
64	Heat transport in epoxy networks: A molecular dynamics study. Polymer, 2009, 50, 3378-3385.	1.8	74
65	Molecular Origin of Solvent Resistance of Polyacrylonitrile. Macromolecules, 2009, 42, 7103-7107.	2.2	44
66	Coarse-grained molecular dynamics simulations of ionic polymer networks. Mechanics of Time-Dependent Materials, 2008, 12, 205-220.	2.3	10
67	A Molecular Dynamics Study of Epoxy-Based Networks: Cross-Linking Procedure and Prediction of Molecular and Material Properties. Macromolecules, 2008, 41, 6837-6842.	2.2	377
68	How does the coupling of secondary and tertiary interactions control the folding of helical macromolecules?. Journal of Chemical Physics, 2007, 126, 044906.	1.2	7
69	A Monte Carlo simulation study of the mechanical and conformational properties of networks of helical polymers. I. General concepts. Polymer, 2005, 46, 3809-3817.	1.8	12
70	Coupling between Helix-Coil and Coil-Globule Transitions in Helical Polymers. Physical Review Letters, 2005, 95, 168304.	2.9	13
71	Stretching Helical Semiflexible Polymers. Macromolecules, 2005, 38, 780-787.	2.2	18
72	A Minimal Model for the Helixâ^'Coil Transition of Wormlike Polymers. Insights from Monte Carlo Simulations and Theoretical Implications. Macromolecules, 2004, 37, 8794-8804.	2.2	19

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73	Structure of Poly(methyl methacrylate) Chains Adsorbed on Sapphire Probed Using Infraredâ˘'Visible Sum Frequency Generation Spectroscopy. Langmuir, 2004, 20, 7183-7188.	1.6	49