

Vikas Varshney

List of Publications by Year in descending order

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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	Thermal properties of graphene: Fundamentals and applications. MRS Bulletin, 2012, 37, 1273-1281.	1.7	1,309
2	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
3	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
4	Preparation of Tunable 3D Pillared Carbon Nanotube-Graphene Networks for High-Performance Capacitance. Chemistry of Materials, 2011, 23, 4810-4816.	3.2	367
5	Emerging Applications of Elemental 2D Materials. Advanced Materials, 2020, 32, e1904302.	11.1	336
6	Modeling of Thermal Transport in Pillared-Graphene Architectures. ACS Nano, 2010, 4, 1153-1161.	7.3	280
7	MD simulations of molybdenum disulphide (MoS ₂): Force-field parameterization and thermal transport behavior. Computational Materials Science, 2010, 48, 101-108.	1.4	158
8	Hydrogenation of Penta-Graphene Leads to Unexpected Large Improvement in Thermal Conductivity. Nano Letters, 2016, 16, 3925-3935.	4.5	142
9	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
10	Nanoscale TiO ₂ films and their application in remediation of organic pollutants. Coordination Chemistry Reviews, 2016, 306, 43-64.	9.5	121
11	Thermal Conductivity of Wurtzite Zinc-Oxide from First-Principles Lattice Dynamics – a Comparative Study with Gallium Nitride. Scientific Reports, 2016, 6, 22504.	1.6	119
12	How to characterize thermal transport capability of 2D materials fairly? – Sheet thermal conductance and the choice of thickness. Chemical Physics Letters, 2017, 669, 233-237.	1.2	103
13	Modeling of Thermal Conductance at Transverse CNT-CNT Interfaces. Journal of Physical Chemistry C, 2010, 114, 16223-16228.	1.5	80
14	Heat transport in epoxy networks: A molecular dynamics study. Polymer, 2009, 50, 3378-3385.	1.8	74
15	Polytypism in ultrathin tellurium. 2D Materials, 2019, 6, 015013.	2.0	68
16	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
17	Thermal Rectification in Three-Dimensional Asymmetric Nanostructure. Nano Letters, 2012, 12, 3491-3496.	4.5	66
18	Molecular Modeling of Cross-Linked Polymers with Complex Cure Pathways: A Case Study of Bismaleimide Resins. Macromolecules, 2018, 51, 1830-1840.	2.2	64

#	ARTICLE	IF	CITATIONS
19	Thermal anisotropy in nano-crystalline MoS ₂ thin films. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 1008-1014.	1.3	63
20	Prediction of 3D elastic moduli and Poisson's ratios of pillared graphene nanostructures. <i>Carbon</i> , 2012, 50, 603-611.	5.4	59
21	Benchmarking Machine Learning Models for Polymer Informatics: An Example of Glass Transition Temperature. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5395-5413.	2.5	59
22	Structure of Poly(methyl methacrylate) Chains Adsorbed on Sapphire Probed Using Infrared-Visible Sum Frequency Generation Spectroscopy. <i>Langmuir</i> , 2004, 20, 7183-7188.	1.6	49
23	Vitrimer Transition Temperature Identification: Coupling Various Thermomechanical Methodologies. <i>ACS Applied Polymer Materials</i> , 2021, 3, 1756-1766.	2.0	47
24	Molecular Origin of Solvent Resistance of Polyacrylonitrile. <i>Macromolecules</i> , 2009, 42, 7103-7107.	2.2	44
25	In situ mechanical investigation of carbon nanotube-graphene junction in three-dimensional carbon nanostructures. <i>Nanoscale</i> , 2017, 9, 2916-2924.	2.8	41
26	Single mode phonon scattering at carbon nanotube-graphene junction in pillared graphene structure. <i>Applied Physics Letters</i> , 2012, 100, 183111.	1.5	36
27	Molecular dynamics simulations of thermal transport in porous nanotube network structures. <i>Nanoscale</i> , 2011, 3, 3679.	2.8	31
28	Transesterification in Vitrimer Polymers Using Bifunctional Catalysts: Modeled with Solution-Phase Experimental Rates and Theoretical Analysis of Efficiency and Mechanisms. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2411-2424.	1.2	30
29	Effect of Curing and Functionalization on the Interface Thermal Conductance in Carbon Nanotube-Epoxy Composites. <i>Jom</i> , 2013, 65, 140-146.	0.9	29
30	Modeling the Role of Bulk and Surface Characteristics of Carbon Fiber on Thermal Conductance across the Carbon-Fiber/Matrix Interface. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 26674-26683.	4.0	25
31	Modeling of interface thermal conductance in longitudinally connected carbon nanotube junctions. <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	24
32	Thermal Reshaping Dynamics of Gold Nanorods: Influence of Size, Shape, and Local Environment. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 43865-43873.	4.0	23
33	Scaling law for energy bandgap and effective electron mass in graphene nano mesh. <i>Applied Physics Letters</i> , 2013, 102, 203107.	1.5	22
34	Creep Mechanics of Epoxy Vitrimer Materials. <i>ACS Applied Polymer Materials</i> , 2022, 4, 4254-4263.	2.0	21
35	Calculation of specific heat of polymers using molecular dynamics simulations. <i>Polymer</i> , 2019, 167, 176-181.	1.8	20
36	A Minimal Model for the Helix-Coil Transition of Wormlike Polymers. Insights from Monte Carlo Simulations and Theoretical Implications. <i>Macromolecules</i> , 2004, 37, 8794-8804.	2.2	19

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37	2D Heterostructure coatings of hBN-MoS_2 layers for corrosion resistance. Journal of Physics D: Applied Physics, 2017, 50, 045301.	1.3	19
38	Stretching Helical Semiflexible Polymers. Macromolecules, 2005, 38, 780-787.	2.2	18
39	Effects of Titanium-Containing Additives on the Dehydrogenation Properties of LiAlH_4 : A Computational and Experimental Study. Journal of Physical Chemistry C, 2012, 116, 22327-22335.	1.5	18
40	A novel nano-configuration for thermoelectrics: helicity induced thermal conductivity reduction in nanowires. Nanoscale, 2012, 4, 5009.	2.8	18
41	Understanding thermal conductance across multi-wall carbon nanotube contacts: Role of nanotube curvature. Carbon, 2017, 114, 15-22.	5.4	18
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	Modeling for predicting strength of carbon nanostructures. Carbon, 2015, 95, 181-189.	5.4	17
44	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
45	Machine learning strategies for the structure-property relationship of copolymers. IScience, 2022, 25, 104585.	1.9	16
46	Bond saturation significantly enhances thermal energy transport in two-dimensional pentagonal materials. Nano Energy, 2018, 45, 1-9.	8.2	15
47	Coupling between Helix-Coil and Coil-Globule Transitions in Helical Polymers. Physical Review Letters, 2005, 95, 168304.	2.9	13
48	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
49	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
50	Single mode phonon energy transmission in functionalized carbon nanotubes. Journal of Chemical Physics, 2011, 135, 104109.	1.2	12
51	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
52	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
53	Multiphysics characterization of multi-walled carbon nanotube thermoplastic polyurethane polymer nanocomposites during compression. Carbon, 2016, 98, 638-648.	5.4	11
54	Molecular dynamics simulations of separator-cathode interfacial thermal transport in a Li-ion cell. Surfaces and Interfaces, 2020, 21, 100674.	1.5	11

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55	Coarse-grained molecular dynamics simulations of ionic polymer networks. <i>Mechanics of Time-Dependent Materials</i> , 2008, 12, 205-220.	2.3	10
56	Thermal interface tailoring in composite materials. <i>Diamond and Related Materials</i> , 2010, 19, 268-272.	1.8	9
57	Modeling of cross-plane interface thermal conductance between graphene nano-ribbons. <i>2D Materials</i> , 2014, 1, 025005.	2.0	9
58	In silico carbon molecular beam epitaxial growth of graphene on the h-BN substrate: carbon source effect on van der Waals epitaxy. <i>Nanoscale</i> , 2016, 8, 9704-9713.	2.8	9
59	Embedded optical nanosensors for monitoring the processing and performance of polymer matrix composites. <i>Journal of Materials Chemistry C</i> , 2019, 7, 14471-14492.	2.7	9
60	Heat Transfer at Aluminum-Water Interfaces: Effect of Surface Roughness. <i>Journal of Nanotechnology in Engineering and Medicine</i> , 2012, 3, .	0.8	8
61	How does the coupling of secondary and tertiary interactions control the folding of helical macromolecules?. <i>Journal of Chemical Physics</i> , 2007, 126, 044906.	1.2	7
62	Developing nanotube junctions with arbitrary specifications. <i>Nanoscale</i> , 2018, 10, 403-415.	2.8	7
63	Breaking the bottleneck: stilbene as a model compound for optimizing π photocyclization efficiency. <i>RSC Advances</i> , 2021, 11, 6504-6508.	1.7	3
64	Temperature dependence of thermal conductance between aluminum and water. <i>International Journal of Thermal Sciences</i> , 2012, 59, 17-20.	2.6	2
65	Computer-aided design of three terminal (3T-) zig-zag SWCNT junctions and nanotube architectures. <i>Composites Science and Technology</i> , 2018, 166, 36-45.	3.8	2
66	A study on mechanical strength and stability of partially-fused carbon nanotube junctions. <i>Carbon Trends</i> , 2021, 3, 100039.	1.4	2
67	Modeling of Mechanical Behavior of Pillard Graphene Structures. , 2010, , .		1
68	Heat Transfer at Aluminum-Water Interfaces: Effect of Surface Roughness. , 2012, , .		1
69	Multi-Terminal Nanotube Junctions: Modeling and Structure-Property Relationship. <i>Frontiers in Materials</i> , 2021, 8, .	1.2	1
70	How does CNT Functionalization and Epoxy Curing affects the Thermal Interface Conductance in CNT-Epoxy Composites? An atomistic modeling perspective. , 2012, , .		0
71	Helicity induced thermal conductivity reduction in superlattice nanowires. , 2012, , .		0
72	Molecular modeling for predicting material and junction strengths of various carbon nanostructures. , 2021, , 67-102.		0

#	ARTICLE	IF	CITATIONS
73	Molecular dynamics methodologies for predicting thermal transport in aerospace polymers and their composites. , 2021, , 19-34.		0