Avinash Parashar

List of Publications by Year
in descending order

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79 papers	2,305 citations	236612 25 h-index	243296 44 g-index
79 all docs	79 docs citations	79 times ranked	989 citing authors

#	Article	IF	Citations
1	Effect of grain boundaries on the interfacial behaviour of graphene-polyethylene nanocomposite. Applied Surface Science, 2019, 470, 1085-1092.	3.1	108
2	Experimental and Computational Studies to Analyze the Effect of h-BN Nanosheets on Mechanical Behavior of h-BN/Polyethylene Nanocomposites. Journal of Physical Chemistry C, 2019, 123, 20059-20070.	1.5	103
3	Effect of Point and Line Defects on Mechanical and Thermal Properties of Graphene: A Review. Critical Reviews in Solid State and Materials Sciences, 2016, 41, 47-71.	6.8	100
4	Atomistic modeling of graphene/hexagonal boron nitride polymer nanocomposites: a review. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1346.	6.2	99
5	Enhanced thermal transport across a bi-crystalline grapheneâ€“polymer interface: an atomistic approach. Physical Chemistry Chemical Physics, 2019, 21, 6229-6237.	1.3	95
6	The effect of STW defects on the mechanical properties and fracture toughness of pristine and hydrogenated graphene. Physical Chemistry Chemical Physics, 2017, 19, 16023-16037.	1.3	89
7	Tersoff potential with improved accuracy for simulating graphene in molecular dynamics environment. Materials Research Express, 2016, 3, 035011.	0.8	85
8	Molecular dynamics based simulations to study failure morphology of hydroxyl and epoxide functionalised graphene. Computational Materials Science, 2018, 143, 15-26.	1.4	84
9	Atomistic modeling of BN nanofillers for mechanical and thermal properties: a review. Nanoscale, 2016, 8, 22-49.	2.8	82
10	Molecular dynamics based simulations to study the fracture strength of monolayer graphene oxide. Nanotechnology, 2018, 29, 115706.	1.3	82
11	Tailoring the failure morphology of 2D bicrystalline graphene oxide. Journal of Applied Physics, 2018, 124, .	1.1	73
12	Representative volume element to estimate buckling behavior of graphene/polymer nanocomposite. Nanoscale Research Letters, 2012, 7, 515.	3.1	71
13	Structural and chemical insights into thermal transport for strained functionalised graphene: a molecular dynamics study. Materials Research Express, 2018, 5, 115605.	0.8	62
14	Optimised cut-off function for Tersoff-like potentials for a BN nanosheet: a molecular dynamics study. Nanotechnology, 2016, 27, 085706.	1.3	59
15	Reactive force field based atomistic simulations to study fracture toughness of bicrystalline graphene functionalised with oxide groups. Diamond and Related Materials, 2018, 88, 193-203.	1.8	58
16	A molecular dynamics based study to estimate the point defects formation energies in graphene containing STW defects. Materials Research Express, 2019, 6, 015606.	0.8	53
17	Adhesively bonded composite tubular joints: Review. International Journal of Adhesion and Adhesives, 2012, 38, 58-68.	1.4	44
18	Effects of Different Hydrogenation Regimes on Mechanical Properties of h-BN: A Reactive Force Field Study. Journal of Physical Chemistry C, 2016, 120, 21932-21938.	1.5	40

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19	Surface Modification Techniques for the Preparation of Different Novel Biofibers for Composites. , 2020, , 1-34.		37
20	Atomistic simulations to study crack tip behaviour in single crystal of bcc niobium and hcp zirconium. Current Applied Physics, 2019, 19, 37-43.	1.1	36
21	Enhancement of fracture toughness of graphene via crack bridging with stone-thrower-wales defects. Diamond and Related Materials, 2017, 74, 90-99.	1.8	33
22	A review on thermo-mechanical properties of bi-crystalline and polycrystalline 2D nanomaterials. Critical Reviews in Solid State and Materials Sciences, 2020, 45, 134-170.	6.8	31
23	Role of Chemical Adatoms in Fracture Mechanics of Graphene Nanolayer. Materials Today: Proceedings, 2019, 11, 920-924.	0.9	30
24	Effect of geometrical defects and functionalization on the interfacial strength of h-BN/polyethylene based nanocomposite. Polymer, 2018, 146, 82-90.	1.8	29
25	Defect dynamics and uniaxial tensile deformation of equi and non-equi-atomic configuration of multi-elemental alloys. Materials Chemistry and Physics, 2021, 266, 124549.	2.0	29
26	Effect of symmetric and asymmetric tilt grain boundaries on the tensile behaviour of bcc-Niobium. Computational Materials Science, 2018, 143, 126-132.	1.4	28
27	Atomistic simulations to study crack tip behaviour in multi-elemental alloys. Engineering Fracture Mechanics, 2021, 243, 107536.	2.0	28
28	Fracture toughness enhancement of h-BN monolayers via hydrogen passivation of a crack edge. Nanotechnology, 2017, 28, 165702.	1.3	27
29	Molecular dynamics study on the mechanical response and failure behaviour of graphene: performance enhancement via 5â€“7â€“7â€–5 defects. RSC Advances, 2016, 6, 26361-26373.	1.7	25
30	Dislocation assisted crack healing in h-BN nanosheets. Physical Chemistry Chemical Physics, 2017, 19, 21739-21747.	1.3	24
31	Effect of symmetrical and asymmetrical tilt grain boundaries on the tensile deformation of zirconium bicrystals: a MD-based study. Journal of Materials Science, 2019, 54, 3082-3095.	1.7	24
32	Effect of Hexagonal Boron Nitride Nanoplatelet on Crystal Nucleation, Mechanical Behavior, and Thermal Stability of Highâ€Density Polyetheleneâ€Based Nanocomposites. Macromolecular Materials and Engineering, 2020, 305, 2000248.	1.7	23
33	Atomistic simulations to study the effect of water molecules on the mechanical behavior of functionalized and non-functionalized boron nitride nanosheets. Computational Materials Science, 2019, 169, 109092.	1.4	22
34	Effect of lattice distortion and nanovoids on the shock compression behavior of (Co-Cr-Cu-Fe-Ni) high entropy alloy. Computational Materials Science, 2022, 209, 111402.	1.4	22
35	Atomistic simulations to study the effect of grain boundaries and hydrogen functionalization on the fracture toughness of bi-crystalline h-BN nanosheets. Physical Chemistry Chemical Physics, 2019, 21, 13116-13125.	1.3	21
36	Mechanical and fracture behavior of water submerged graphene. Journal of Applied Physics, 2019, 125, 215107.	1.1	21

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37	Inter-granular fracture toughness of bi-crystalline graphene nanosheets. Diamond and Related Materials, 2020, 102, 107667.	1.8	21
38	Characterization of 2D Nanomaterials for Energy Storage. Lecture Notes in Mechanical Engineering, 2020, , 221-226.	0.3	21
39	Molecular dynamics based study of an irradiated single crystal of niobium. Computational Materials Science, 2017, 131, 48-54.	1.4	20
40	Mechanical strength of a nanoporous bicrystalline h-BN nanomembrane in a water submerged state. Physical Chemistry Chemical Physics, 2020, 22, 20453-20465.	1.3	19
41	Polymer-based nanocomposites for impact loading: A review. Mechanics of Advanced Materials and Structures, 2022, 29, 2581-2606.	1.5	19
42	Atomistic simulations to study the effect of helium nanobubble on the shear deformation of nickel crystal. Journal of Nuclear Materials, 2021, 557, 153245.	1.3	19
43	Multiscale Model to Study of Fracture Toughening in Graphene/Polymer Nanocomposite. International Journal of Fracture, 2013, 179, 221-228.	1.1	18
44	Molecular dynamics-based simulations to study crack tip interaction with symmetrical and asymmetrical tilt grain boundaries in Zr. Journal of Nuclear Materials, 2019, 526, 151739.	1.3	18
45	Lifecycle Assessment of Thermoplastic and Thermosetting Bamboo Composites. , 2021, , 235-246.		18
46	Effect of symmetrical and asymmetrical tilt grain boundaries on radiation-induced defects in zirconium. Journal Physics D: Applied Physics, 2018, 51, 265301.	1.3	17
47	Mechanical and fracture behaviour of hydroxyl functionalized h-BN nanosheets. Journal of Materials Science, 2020, 55, 3228-3242.	1.7	17
48	Experimental and atomistic insight on the thermal transport properties of h-BN/high density polyethylene nanocomposite. International Journal of Heat and Mass Transfer, 2021, 170, 121039.	2.5	17
49	Multiscale model to investigate the effect of graphene on the fracture characteristics of graphene/polymer nanocomposites. Nanoscale Research Letters, 2012, 7, 595.	3.1	16
50	An atomistic approach to study the dynamic and structural response in 2D nanofiller reinforced polyethylene nanocomposites under ultra-short shock pulse loading. Mechanics of Materials, 2022, 169, 104305.	1.7	14
51	Deformation dynamics of h-BN reinforced polyethylene nanocomposite under shock/impact loading. International Journal of Mechanical Sciences, 2022, 225, 107379.	3.6	14
52	Defect formation dynamics in dry and water submerged graphene nanosheets. Materials Research Express, 2019, 6, 075063.	0.8	12
53	Study of Mode I Fracture of Graphene Sheets Using Atomistic Based Finite Element Modeling and Virtual Crack Closure Technique. International Journal of Fracture, 2012, 176, 119-126.	1.1	11
54	Molecular Dynamics Study of Anisotropic Shock Response in Mono- and Bicrystalline Boron Nitride Nanosheets: Implications for Shock-Resistant Solid-State Devices. ACS Applied Nano Materials, 2022, 5, 2787-2800.	2.4	11

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55	Anisotropic compressive response of Stoneâ€“Throwerâ€“Wales defects in graphene: A molecular dynamics study. Materials Research Express, 2016, 3, 095015.	0.8	10
56	Displacement thresholds and knock-on cross sections for hydrogenated h-BN monolayers. Computational Materials Science, 2018, 142, 82-88.	1.4	10
57	Effect of non-bonded interactions on failure morphology of a defective graphene sheet. Materials Research Express, 2016, 3, 045009.	0.8	9
58	Atomistic simulations to study point defect dynamics in bi-crystalline niobium. Materials Chemistry and Physics, 2020, 255, 123628.	2.0	9
59	Effect of van der Waals interaction on the mode I fracture characteristics of graphene sheet. Solid State Communications, 2013, 173, 56-60.	0.9	8
60	Finite Element Analysis to Study the Effect of Dimensional and Geometrical Parameters on the Stability of Graphene Sheets. Journal of Computational and Theoretical Nanoscience, 2013, 10, 292-298.	0.4	8
61	Effect of topological defects on mechanical properties of graphene sheets: a molecular dynamics study. Materials Today: Proceedings, 2018, 5, 6780-6788.	0.9	7
62	Atomistic scale insight to investigate the strain rate effect on mechanical response of boron nitride nanosheet reinforced nanocomposites. Materials Today: Proceedings, 2022, 62, 7523-7527.	0.9	7
63	Effect of Nb precipitate on defect formation and migration energies in bi-crystalline Zr. Materials Chemistry and Physics, 2019, 235, 121729.	2.0	6
64	Atomistic simulations to study the effect of Nb precipitate on fracture properties of bi-crystalline Zr. Journal Physics D: Applied Physics, 2019, 52, 355304.	1.3	6
65	Enhancement in Mechanical Properties of Polyethylene Using h-BN Nanofiller. Lecture Notes in Mechanical Engineering, 2021, , 127-133.	0.3	6
66	Effect of BNNR on mechanical properties of polyethylene nanocomposites. Materials Today: Proceedings, 2021, 47, 2875-2877.	0.9	6
67	Atomistic simulations to study shock and ultrashort pulse response of high entropy alloy. Materials Today: Proceedings, 2022, 62, 7494-7500.	0.9	6
68	Inter-granular fracture behaviour in bicrystalline boron nitride nanosheets using atomistic and continuum mechanics-based approaches. Journal of Materials Science, 2021, 56, 6235-6250.	1.7	5
69	Atomistic simulations to study the effects of helium bubbles on crack tip behavior in single crystal Ni. Journal Physics D: Applied Physics, 2021, 54, 365305.	1.3	4
70	Evaluation of Interfacial Shear Strength of h-BN/PE Nanocomposites Using Molecular Dynamics. Lecture Notes in Mechanical Engineering, 2021, , 105-113.	0.3	4
71	Fracture behaviour of pristine and defective form of water submerged h-BN nanosheets. Journal Physics D: Applied Physics, 2021, 54, 035306.	1.3	4
72	Effect of van der Waals Forces on the Buckling Strength of Graphene. Journal of Computational and Theoretical Nanoscience, 2013, 10, 2626-2630.	0.4	3

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73	Sequential multiscale model to study crack tip behavior in bi-crystalline graphene. Journal of Applied Physics, 2020, 127, 225103.	1.1	3
74	A Comparison between â˜3 Asymmetrical Tilt Grain Boundary Energies in Niobium Obtained Analytically and through Molecular Dynamics Based Simulations. Materials Science Forum, 2020, 998, 179-184.	0.3	2
75	Effect of Crack on the Tensile Strength of a Bicrystal Zr - A MD Based Evaluation. Materials Science Forum, 2020, 978, 487-491.	0.3	2
76	Fracture Toughness Enhancement of Boron Nitride Nanosheets via Crack Edge Passivation Using Various Radicals. Lecture Notes in Mechanical Engineering, 2021, , 111-117.	0.3	1
77	Effect of symmetrical tilt grain boundary on dislocation nucleation and growth in Niobium bi-crystal. Materials Today: Proceedings, 2019, 11, 925-928.	0.9	0
78	Effect of defects and functionalization on mechanical and fracture properties of two-dimensional nanomaterials. , 2021, , 543-567.		0
79	Enhanced Mechanical Properties of h-BN Nanosheets via Edge Passivation Using Various Radicals. Lecture Notes in Mechanical Engineering, 2021, , 97-103.	0.3	0