

Shahram Ajori

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

76
papers

1,122
citations

21
h-index

30
g-index

76
ext. papers

1,210
ext. citations

2.6
avg, IF

5.22
L-index

#	Paper	IF	Citations
76	Mechanical properties and fracture analysis of defective penta-graphene under temperature variation: Insight from molecular dynamics. <i>Diamond and Related Materials</i> , 2022 , 124, 108956	3.5	0
75	Effect of defects and boundary conditions on the vibrational behavior of carbon nanotube and graphene: A molecular dynamics perspective. <i>Diamond and Related Materials</i> , 2022 , 126, 109052	3.5	0
74	High velocity impact analysis of free-free carbon nanotubes.. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 111, 108105	2.8	
73	Fundamental frequency analysis of endohedrally functionalized carbon nanotubes with metallic nanowires: a molecular dynamics study. <i>Journal of Molecular Modeling</i> , 2021 , 27, 313	2	1
72	A molecular dynamics study on the buckling behavior of x-graphyne based single- and multi-walled nanotubes. <i>Computational Materials Science</i> , 2021 , 191, 110333	3.2	4
71	A molecular dynamics study on the tensile characteristics of various metallic glass nanocomposites reinforced by Weyl semimetals three-dimensional graphene network. <i>European Journal of Mechanics, A/Solids</i> , 2021 , 85, 104104	3.7	5
70	Thermal conductivity of three-dimensional metallic carbon nanostructures (T6) with boron and nitrogen dopant. <i>European Physical Journal D</i> , 2020 , 74, 1	1.3	1
69	Stacking Interactions of Poly Para-Phenylene Vinylene Oligomers with Graphene and Single-Walled Carbon Nanotubes: A Molecular Dynamics Approach. <i>Molecules</i> , 2020 , 25,	4.8	1
68	Characterizing the mechanical properties and fracture pattern of defective hexagonal boron-nitride sheets with focus on Stone-Wales defect. <i>Superlattices and Microstructures</i> , 2020 , 142, 106526	2.8	4
67	Effect of metallic nanowire encapsulation on the tensile behavior of single-walled carbon nanotubes: a molecular dynamics study. <i>European Physical Journal D</i> , 2020 , 74, 1	1.3	3
66	Interfacial characteristics and thermo-mechanical properties of calcium carbonate/polystyrene nanocomposite. <i>Materials Chemistry and Physics</i> , 2020 , 247, 122871	4.4	8
65	A molecular dynamics study on the buckling behavior of single-walled carbon nanotubes filled with gold nanowires. <i>Journal of Molecular Modeling</i> , 2020 , 26, 196	2	3
64	Adsorption analysis and mechanical characteristics of carbon nanotubes under physisorption of biological molecules in an aqueous environment using molecular dynamics simulations. <i>Molecular Simulation</i> , 2020 , 46, 388-397	2	5
63	The adsorption characteristics and thermo-mechanical properties of BxCyNz heteronanotubes under physical adsorption of Ni(II)-tetramethyldibenzotetraaza[14]annulene (NiTMTAA): Insight from molecular dynamics approach. <i>Computational Materials Science</i> , 2020 , 176, 109554	3.2	4
62	A comprehensive analysis of the mechanical properties and fracture analysis of metallic glass nanocomposites reinforced by carbon nanotubes and Cu nanowires: A molecular dynamics study. <i>Mechanics of Advanced Materials and Structures</i> , 2020 , 1-20	1.8	5
61	The effect of chitosan adsorption on the stability characteristics of single- and double-walled boron-nitride nanotubes under compressive force using molecular dynamics simulations. <i>Structural Chemistry</i> , 2020 , 31, 909-915	1.8	1
60	Continuum modeling of ion-selective membranes constructed from functionalized carbon nanotubes. <i>European Physical Journal Plus</i> , 2020 , 135, 1	3.1	7

59	Fracture analysis and tensile properties of perfect and defective carbon nanotubes functionalized with carbene using molecular dynamics simulations. <i>Journal of the Brazilian Society of Mechanical Sciences and Engineering</i> , 2020 , 42, 1	2	7
58	Nano-oscillators based on a C60 fullerene inside open carbon nanocones: a molecular dynamics study. <i>Journal of the Brazilian Society of Mechanical Sciences and Engineering</i> , 2020 , 42, 1	2	0
57	A molecular dynamics study on the interfacial properties of carbene-functionalized graphene/polymer nanocomposites. <i>International Journal of Mechanics and Materials in Design</i> , 2020 , 16, 387-400	2.5	9
56	On the buckling behavior of functionalized single- and double-walled carbon nanotubes with azobenzene in the aqueous environment: a molecular dynamics study. <i>Structural Chemistry</i> , 2020 , 31, 371-384	1.8	
55	Characterization of the structural instability of BxCyNz heteronanotubes via molecular dynamics simulations. <i>Materials Research Express</i> , 2019 , 6, 105096	1.7	6
54	Interfacial properties of 3D metallic carbon nanostructures (T6 and T14)-reinforced polymer nanocomposites: A molecular dynamics study. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 92, 341-356	2.8	11
53	On the mechanical stability and buckling analysis of carbon nanotubes filled with ice nanotubes in the aqueous environment: A molecular dynamics simulation approach. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 89, 74-81	2.8	12
52	Small strain effect on the mechanical vibration behavior of cross-linked functionalized carbon nanotubes with polyethylene: A molecular-dynamics study. <i>Europhysics Letters</i> , 2019 , 125, 43001	1.6	10
51	Influence of polyethylene cross-linked functionalization on the interfacial properties of carbon nanotube-reinforced polymer nanocomposites: a molecular dynamics study. <i>Journal of Molecular Modeling</i> , 2019 , 25, 105	2	13
50	Structural properties and buckling behavior of non-covalently functionalized single- and double-walled carbon nanotubes with pyrene-linked polyamide in aqueous environment using molecular dynamics simulations. <i>Journal of Physics and Chemistry of Solids</i> , 2019 , 131, 79-85	3.9	15
49	The mechanical properties and structural instability of single- and double-walled boron-nitride nanotubes functionalized with 2-methoxy-N,N-dimethylethanamine (MDE) using molecular dynamics simulations. <i>European Physical Journal D</i> , 2019 , 73, 1	1.3	6
48	Buckling behavior of various metallic glass nanocomposites reinforced by carbon nanotube and Cu nanowire: A molecular dynamics simulation study. <i>Materials Research Express</i> , 2019 , 6, 095070	1.7	14
47	Tensile characteristics of carbene-functionalized CNTs subjected to physisorption of polymer chains: a molecular dynamics study. <i>Journal of Molecular Modeling</i> , 2019 , 25, 318	2	9
46	Tensile characteristics of single-walled carbon nanotubes endohedrally decorated with gold nanowires: A molecular dynamics study. <i>Diamond and Related Materials</i> , 2019 , 92, 117-129	3.5	13
45	Stability analysis of endohedrally functionalized carbon nanotubes with pentagonal metallic nanowires: a molecular dynamics simulation approach. <i>Materials Research Express</i> , 2019 , 6, 045056	1.7	6
44	A molecular dynamics study on the thermal conductivity of endohedrally functionalized single-walled carbon nanotubes with gold nanowires. <i>European Physical Journal D</i> , 2018 , 72, 1	1.3	21
43	Molecular dynamics simulations of the polymer/amine functionalized single-walled carbon nanotubes interactions. <i>Applied Surface Science</i> , 2018 , 455, 171-180	6.7	15
42	Molecular dynamics simulations of the thermal conductivity of cross-linked functionalized single- and double-walled carbon nanotubes with polyethylene chains. <i>Diamond and Related Materials</i> , 2018 , 86, 173-178	3.5	21

41	A molecular dynamics study on the buckling behavior of cross-linked functionalized carbon nanotubes under physical adsorption of polymer chains. <i>Applied Surface Science</i> , 2018 , 427, 704-714	6.7	22
40	Vibrational analysis of single-walled carbon nanotubes filled with gold nanowires using MD simulations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018 , 104, 327-332	3	9
39	Molecular dynamics study of gigahertz nanomechanical oscillators based on an ion inside a series of electrically charged carbon nanotubes. <i>European Journal of Mechanics, A/Solids</i> , 2018 , 69, 45-54	3.7	18
38	Structural stability and buckling analysis of a series of carbon nanotorus using molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2018 , 24, 263	2	1
37	Vibration characteristics of three-dimensional metallic carbon nanostructures with interlocking hexagons pattern (T6 and T14): A molecular dynamics study. <i>Computational Materials Science</i> , 2017 , 128, 81-86	3.2	6
36	Buckling Behavior of Carbon Nanotubes Functionalized with Carbene under Physical Adsorption of Polymer Chains: a Molecular Dynamics Study. <i>Brazilian Journal of Physics</i> , 2017 , 47, 606-616	1.2	5
35	Oscillation characteristics of carbon nanotori molecules along carbon nanotubes under various system parameters. <i>European Journal of Mechanics, A/Solids</i> , 2017 , 62, 67-79	3.7	12
34	A molecular dynamics investigation into the size-dependent buckling behavior of a novel three-dimensional metallic carbon nanostructure (T6). <i>Superlattices and Microstructures</i> , 2016 , 97, 125-131	2.8	4
33	Stability characteristics and structural properties of single- and double-walled boron-nitride nanotubes under physical adsorption of Flavin mononucleotide (FMN) in aqueous environment using molecular dynamics simulations. <i>Applied Surface Science</i> , 2016 , 366, 233-244	6.7	22
32	On the vibrational behavior of single- and double-walled carbon nanotubes under the physical adsorption of biomolecules in the aqueous environment: a molecular dynamics study. <i>Journal of Molecular Modeling</i> , 2016 , 22, 62	2	12
31	Characterization of the mechanical properties of polyphenylene polymer using molecular dynamics simulations. <i>Physica B: Condensed Matter</i> , 2016 , 481, 80-85	2.8	10
30	Buckling analysis of defective cross-linked functionalized single- and double-walled carbon nanotubes with polyethylene chains using molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2016 , 22, 298	2	3
29	Prediction of structural and mechanical properties of atom-decorated porous graphene via density functional calculations. <i>EPJ Applied Physics</i> , 2016 , 74, 10401	1.1	11
28	On the Interfacial Properties of Polymers/Functionalized Single-Walled Carbon Nanotubes. <i>Brazilian Journal of Physics</i> , 2016 , 46, 361-369	1.2	8
27	Molecular dynamics investigation into the oscillatory behavior of double-walled boron-nitride nanotubes. <i>Superlattices and Microstructures</i> , 2016 , 93, 18-26	2.8	12
26	Influence of Electric Field on the Mechanical Properties of Hexagonal Boron-Nitride Sheets Using ab-initio Calculations. <i>Nano</i> , 2015 , 10, 1550047	1.1	6
25	A molecular dynamics study on the vibration of carbon and boron nitride double-walled hybrid nanotubes. <i>Applied Physics A: Materials Science and Processing</i> , 2015 , 120, 1399-1406	2.6	26
24	On the vibrational characteristics of single- and double-walled carbon nanotubes containing ice nanotube in aqueous environment. <i>Applied Physics A: Materials Science and Processing</i> , 2015 , 121, 223-232	2.6	14

23	Investigation of the adsorption of polymer chains on amine-functionalized double-walled carbon nanotubes. <i>Journal of Molecular Modeling</i> , 2015 , 21, 312	2	10
22	Vibrational characteristics of diethyltoluenediamines (DETA) functionalized carbon nanotubes using molecular dynamics simulations. <i>Physica B: Condensed Matter</i> , 2015 , 459, 58-61	2.8	21
21	Elastic properties and buckling behavior of single-walled carbon nanotubes functionalized with diethyltoluenediamines using molecular dynamics simulations. <i>Superlattices and Microstructures</i> , 2015 , 77, 54-63	2.8	32
20	Molecular dynamics investigation into the electric charge effect on the operation of ion-based carbon nanotube oscillators. <i>Journal of Physics and Chemistry of Solids</i> , 2015 , 85, 264-272	3.9	27
19	Structural and elastic properties and stability characteristics of oxygenated carbon nanotubes under physical adsorption of polymers. <i>Applied Surface Science</i> , 2015 , 332, 640-647	6.7	36
18	Vibration characteristics of single- and double-walled carbon nanotubes functionalized with amide and amine groups. <i>Physica B: Condensed Matter</i> , 2015 , 462, 8-14	2.8	24
17	Structural and elastic properties of hybrid bilayer graphene/h-BN with different interlayer distances using DFT. <i>Superlattices and Microstructures</i> , 2014 , 72, 230-237	2.8	21
16	Elastic and structural properties and buckling behavior of single-walled carbon nanotubes under chemical adsorption of atomic oxygen and hydroxyl. <i>Chemical Physics Letters</i> , 2014 , 616-617, 120-125	2.5	31
15	Molecular dynamics study of the torsional vibration characteristics of boron-nitride nanotubes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014 , 378, 2876-2880	2.3	23
14	Torsional buckling behavior of boron-nitride nanotubes using molecular dynamics simulations. <i>Current Applied Physics</i> , 2014 , 14, 1072-1077	2.6	22
13	On the Vibration of Single-Walled Carbon Nanocones: Molecular Mechanics Approach versus Molecular Dynamics Simulations. <i>Shock and Vibration</i> , 2014 , 2014, 1-8	1.1	8
12	Elastic properties and large deformation of two-dimensional silicene nanosheets using molecular dynamics. <i>Superlattices and Microstructures</i> , 2014 , 65, 64-70	2.8	34
11	Continuum and molecular dynamics study of C60 fullerene-carbon nanotube oscillators. <i>Mechanics Research Communications</i> , 2013 , 47, 18-23	2.2	36
10	Mechanical properties of defective graphene using molecular dynamics simulations. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2013 , 561, 34-39	5.3	52
9	Structural and elastic properties of carbon nanotubes containing Fe atoms using first principles. <i>Superlattices and Microstructures</i> , 2013 , 64, 220-226	2.8	11
8	Torsional Vibration Analysis of Carbon Nanotubes Based on the Strain Gradient Theory and Molecular Dynamic Simulations. <i>Journal of Vibration and Acoustics, Transactions of the ASME</i> , 2013 , 135,	1.6	27
7	Characterization of the Mechanical Properties of Monolayer Molybdenum Disulfide Nanosheets Using First Principles. <i>Journal of Nanotechnology in Engineering and Medicine</i> , 2013 , 4,		4
6	Mechanical properties of defective single-layered graphene sheets via molecular dynamics simulation. <i>Superlattices and Microstructures</i> , 2012 , 51, 274-289	2.8	137

5	Vibrations of single- and double-walled carbon nanotubes with layerwise boundary conditions: A molecular dynamics study. <i>Current Applied Physics</i> , 2012 , 12, 707-711	2.6	62
4	Fracture analysis of monolayer graphene sheets with double vacancy defects via MD simulation. <i>Solid State Communications</i> , 2011 , 151, 1141-1146	1.6	59
3	Thermal conductivity of perfect and defective carbon nanotubes functionalized with carbene: a molecular dynamics study. <i>Molecular Simulation</i> , 1-9	2	4
2	Molecular dynamics study on the effect of polymer physisorption on the thermal conductivity of cross-linked functionalized carbon nanotubes. <i>Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science</i> , 095440622110424	1.3	0
1	Dynamic behavior of chloride ion-electrically charged open carbon nanocone oscillators: A molecular dynamics study. <i>Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science</i> , 095440622098450	1.3	0