Shahram Ajori

List of Publications by Citations

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 of defective single-layered graphene sheets via molecular dynamics simulation. *Superlattices and Microstructures*, **2012**, 51, 274-289	2.8	137
75	Vibrations of single- and double-walled carbon nanotubes with layerwise boundary conditions: A molecular dynamics study. *Current Applied Physics*, **2012**, 12, 707-711	2.6	62
74	Fracture analysis of monolayer graphene sheets with double vacancy defects via MD simulation. *Solid State Communications*, **2011**, 151, 1141-1146	1.6	59
73	Mechanical properties of defective graphyne using molecular dynamics simulations. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2013**, 561, 34-39	5.3	52
72	Continuum and molecular dynamics study of C60 fullerene–carbon nanotube oscillators. *Mechanics Research Communications*, **2013**, 47, 18-23	2.2	36
71	Structural and elastic properties and stability characteristics of oxygenated carbon nanotubes under physical adsorption of polymers. *Applied Surface Science*, **2015**, 332, 640-647	6.7	36
70	Elastic properties and large deformation of two-dimensional silicene nanosheets using molecular dynamics. *Superlattices and Microstructures*, **2014**, 65, 64-70	2.8	34
69	Elastic properties and buckling behavior of single-walled carbon nanotubes functionalized with diethyltoluenediamines using molecular dynamics simulations. *Superlattices and Microstructures*, **2015**, 77, 54-63	2.8	32
68	Elastic and structural properties and buckling behavior of single-walled carbon nanotubes under chemical adsorption of atomic oxygen and hydroxyl. *Chemical Physics Letters*, **2014**, 616-617, 120-125	2.5	31
67	Molecular dynamics investigation into the electric charge effect on the operation of ion-based carbon nanotube oscillators. *Journal of Physics and Chemistry of Solids*, **2015**, 85, 264-272	3.9	27
66	Torsional Vibration Analysis of Carbon Nanotubes Based on the Strain Gradient Theory and Molecular Dynamic Simulations. *Journal of Vibration and Acoustics, Transactions of the ASME*, **2013**, 135,	1.6	27
65	A molecular dynamics study on the vibration of carbon and boron nitride double-walled hybrid nanotubes. *Applied Physics A: Materials Science and Processing*, **2015**, 120, 1399-1406	2.6	26
64	Vibration characteristics of single- and double-walled carbon nanotubes functionalized with amide and amine groups. *Physica B: Condensed Matter*, **2015**, 462, 8-14	2.8	24
63	Molecular dynamics study of the torsional vibration characteristics of boron-nitride nanotubes. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 2876-2880	2.3	23
62	A molecular dynamics study on the buckling behavior of cross-linked functionalized carbon nanotubes under physical adsorption of polymer chains. *Applied Surface Science*, **2018**, 427, 704-714	6.7	22
61	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. *Applied Surface Science*, **2016**, 366, 233-244	6.7	22
60	Torsional buckling behavior of boron-nitride nanotubes using molecular dynamics simulations. *Current Applied Physics*, **2014**, 14, 1072-1077	2.6	22

59	Vibrational characteristics of diethyltoluenediamines (DETDA) functionalized carbon nanotubes using molecular dynamics simulations. *Physica B: Condensed Matter*, **2015**, 459, 58-61	2.8	21
58	A molecular dynamics study on the thermal conductivity of endohedrally functionalized single-walled carbon nanotubes with gold nanowires. *European Physical Journal D*, **2018**, 72, 1	1.3	21
57	Molecular dynamics simulations of the thermal conductivity of cross-linked functionalized single- and double-walled carbon nanotubes with polyethylene chains. *Diamond and Related Materials*, **2018**, 86, 173-178	3.5	21
56	Structural and elastic properties of hybrid bilayer graphene/h-BN with different interlayer distances using DFT. *Superlattices and Microstructures*, **2014**, 72, 230-237	2.8	21
55	Molecular dynamics study of gigahertz nanomechanical oscillators based on an ion inside a series of electrically charged carbon nanotubes. *European Journal of Mechanics, A/Solids*, **2018**, 69, 45-54	3.7	18
54	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. *Journal of Physics and Chemistry of Solids*, **2019**, 131, 79-85	3.9	15
53	Molecular dynamics simulations of the polymer/amine functionalized single-walled carbon nanotubes interactions. *Applied Surface Science*, **2018**, 455, 171-180	6.7	15
52	On the vibrational characteristics of single- and double-walled carbon nanotubes containing ice nanotube in aqueous environment. *Applied Physics A: Materials Science and Processing*, **2015**, 121, 223-232	2.6	14
51	Buckling behavior of various metallic glass nanocomposites reinforced by carbon nanotube and Cu nanowire: A molecular dynamics simulation study. *Materials Research Express*, **2019**, 6, 095070	1.7	14
50	Influence of polyethylene cross-linked functionalization on the interfacial properties of carbon nanotube-reinforced polymer nanocomposites: a molecular dynamics study. *Journal of Molecular Modeling*, **2019**, 25, 105	2	13
49	Tensile characteristics of single-walled carbon nanotubes endohedrally decorated with gold nanowires: A molecular dynamics study. *Diamond and Related Materials*, **2019**, 92, 117-129	3.5	13
48	On the mechanical stability and buckling analysis of carbon nanotubes filled with ice nanotubes in the aqueous environment: A molecular dynamics simulation approach. *Journal of Molecular Graphics and Modelling*, **2019**, 89, 74-81	2.8	12
47	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. *Journal of Molecular Modeling*, **2016**, 22, 62	2	12
46	Oscillation characteristics of carbon nanotori molecules along carbon nanotubes under various system parameters. *European Journal of Mechanics, A/Solids*, **2017**, 62, 67-79	3.7	12
45	Molecular dynamics investigation into the oscillatory behavior of double-walled boron-nitride nanotubes. *Superlattices and Microstructures*, **2016**, 93, 18-26	2.8	12
44	Interfacial properties of 3D metallic carbon nanostructures (T6 and T14)-reinforced polymer nanocomposites: A molecular dynamics study. *Journal of Molecular Graphics and Modelling*, **2019**, 92, 341-356	2.8	11
43	Structural and elastic properties of carbon nanotubes containing Fe atoms using first principles. *Superlattices and Microstructures*, **2013**, 64, 220-226	2.8	11
42	Prediction of structural and mechanical properties of atom-decorated porous graphene via density functional calculations. *EPJ Applied Physics*, **2016**, 74, 10401	1.1	11

41	Small strain effect on the mechanical vibration behavior of cross-linked functionalized carbon nanotubes with polyethylene: A molecular-dynamics study. *Europhysics Letters*, **2019**, 125, 43001	1.6	10
40	Investigation of the adsorption of polymer chains on amine-functionalized double-walled carbon nanotubes. *Journal of Molecular Modeling*, **2015**, 21, 312	2	10
39	Characterization of the mechanical properties of polyphenylene polymer using molecular dynamics simulations. *Physica B: Condensed Matter*, **2016**, 481, 80-85	2.8	10
38	Vibrational analysis of single-walled carbon nanotubes filled with gold nanowires using MD simulations. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 104, 327-332	3	9
37	Tensile characteristics of carbene-functionalized CNTs subjected to physisorption of polymer chains: a molecular dynamics study. *Journal of Molecular Modeling*, **2019**, 25, 318	2	9
36	A molecular dynamics study on the interfacial properties of carbene-functionalized graphene/polymer nanocomposites. *International Journal of Mechanics and Materials in Design*, **2020**, 16, 387-400	2.5	9
35	Interfacial characteristics and thermo-mechanical properties of calcium carbonate/polystyrene nanocomposite. *Materials Chemistry and Physics*, **2020**, 247, 122871	4.4	8
34	On the Vibration of Single-Walled Carbon Nanocones: Molecular Mechanics Approach versus Molecular Dynamics Simulations. *Shock and Vibration*, **2014**, 2014, 1-8	1.1	8
33	On the Interfacial Properties of Polymers/Functionalized Single-Walled Carbon Nanotubes. *Brazilian Journal of Physics*, **2016**, 46, 361-369	1.2	8
32	Continuum modeling of ion-selective membranes constructed from functionalized carbon nanotubes. *European Physical Journal Plus*, **2020**, 135, 1	3.1	7
31	Fracture analysis and tensile properties of perfect and defective carbon nanotubes functionalized with carbene using molecular dynamics simulations. *Journal of the Brazilian Society of Mechanical Sciences and Engineering*, **2020**, 42, 1	2	7
30	Vibration characteristics of three-dimensional metallic carbon nanostructures with interlocking hexagons pattern (T6 and T14): A molecular dynamics study. *Computational Materials Science*, **2017**, 128, 81-86	3.2	6
29	Characterization of the structural instability of BxCyNz heteronanotubes via molecular dynamics simulations. *Materials Research Express*, **2019**, 6, 105096	1.7	6
28	Influence of Electric Field on the Mechanical Properties of Hexagonal Boron-Nitride Sheets Using ab-initio Calculations. *Nano*, **2015**, 10, 1550047	1.1	6
27	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. *European Physical Journal D*, **2019**, 73, 1	1.3	6
26	Stability analysis of endohedrally functionalized carbon nanotubes with pentagonal metallic nanowires: a molecular dynamics simulation approach. *Materials Research Express*, **2019**, 6, 045056	1.7	6
25	Buckling Behavior of Carbon Nanotubes Functionalized with Carbene under Physical Adsorption of Polymer Chains: a Molecular Dynamics Study. *Brazilian Journal of Physics*, **2017**, 47, 606-616	1.2	5
24	Adsorption analysis and mechanical characteristics of carbon nanotubes under physisorption of biological molecules in an aqueous environment using molecular dynamics simulations. *Molecular Simulation*, **2020**, 46, 388-397	2	5

23	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. *Mechanics of Advanced Materials and Structures*, **2020**, 1-20	1.8	5
22	A molecular dynamics study on the tensile characteristics of various metallic glass nanocomposites reinforced by Weyl semimetals three-dimensional graphene network. *European Journal of Mechanics, A/Solids*, **2021**, 85, 104104	3.7	5
21	Characterizing the mechanical properties and fracture pattern of defective hexagonal boron-nitride sheets with focus on Stone-Wales defect. *Superlattices and Microstructures*, **2020**, 142, 106526	2.8	4
20	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. *Computational Materials Science*, **2020**, 176, 109554	3.2	4
19	A molecular dynamics investigation into the size-dependent buckling behavior of a novel three-dimensional metallic carbon nanostructure (T6). *Superlattices and Microstructures*, **2016**, 97, 125-131	2.8	4
18	Characterization of the Mechanical Properties of Monolayer Molybdenum Disulfide Nanosheets Using First Principles. *Journal of Nanotechnology in Engineering and Medicine*, **2013**, 4,		4
17	A molecular dynamics study on the buckling behavior of x-graphyne based single- and multi-walled nanotubes. *Computational Materials Science*, **2021**, 191, 110333	3.2	4
16	Thermal conductivity of perfect and defective carbon nanotubes functionalized with carbene: a molecular dynamics study. *Molecular Simulation*,1-9	2	4
15	Effect of metallic nanowire encapsulation on the tensile behavior of single-walled carbon nanotubes: a molecular dynamics study. *European Physical Journal D*, **2020**, 74, 1	1.3	3
14	A molecular dynamics study on the buckling behavior of single-walled carbon nanotubes filled with gold nanowires. *Journal of Molecular Modeling*, **2020**, 26, 196	2	3
13	Buckling analysis of defective cross-linked functionalized single- and double-walled carbon nanotubes with polyethylene chains using molecular dynamics simulations. *Journal of Molecular Modeling*, **2016**, 22, 298	2	3
12	Thermal conductivity of three-dimensional metallic carbon nanostructures (T6) with boron and nitrogen dopant. *European Physical Journal D*, **2020**, 74, 1	1.3	1
11	Stacking Interactions of Poly Para-Phenylene Vinylene Oligomers with Graphene and Single-Walled Carbon Nanotubes: A Molecular Dynamics Approach. *Molecules*, **2020**, 25,	4.8	1
10	Fundamental frequency analysis of endohedrally functionalized carbon nanotubes with metallic nanowires: a molecular dynamics study. *Journal of Molecular Modeling*, **2021**, 27, 313	2	1
9	The effect of chitosan adsorption on the stability characteristics of single- and double-walled boron-nitride nanotubes under compressive force using molecular dynamics simulations. *Structural Chemistry*, **2020**, 31, 909-915	1.8	1
8	Structural stability and buckling analysis of a series of carbon nanotorus using molecular dynamics simulations. *Journal of Molecular Modeling*, **2018**, 24, 263	2	1
7	Nano-oscillators based on a C60 fullerene inside open carbon nanocones: a molecular dynamics study. *Journal of the Brazilian Society of Mechanical Sciences and Engineering*, **2020**, 42, 1	2	0
6	Molecular dynamics study on the effect of polymer physisorption on the thermal conductivity of cross-linked functionalized carbon nanotubes. *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*,095440622110424	1.3	0

5	Dynamic behavior of chloride ion-electrically charged open carbon nanocone oscillators: A molecular dynamics study. *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*,095440622098450	1.3	0
4	Mechanical properties and fracture analysis of defective penta-graphene under temperature variation: Insight from molecular dynamics. *Diamond and Related Materials*, **2022**, 124, 108956	3.5	0
3	Effect of defects and boundary conditions on the vibrational behavior of carbon nanotube and graphene: A molecular dynamics perspective. *Diamond and Related Materials*, **2022**, 126, 109052	3.5	0
2	High velocity impact analysis of free-free carbon nanotubes.. *Journal of Molecular Graphics and Modelling*, **2021**, 111, 108105	2.8	
1	On the buckling behavior of functionalized single- and double-walled carbon nanotubes with azobenzene in the aqueous environment: a molecular dynamics study. *Structural Chemistry*, **2020**, 31, 371-384	1.8	