Shahram Ajori

List of Publications by Year
in descending order

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76 papers	1,319 citations	331259 21 h-index	414034 32 g-index
76 all docs	76 docs citations	76 times ranked	959 citing authors

#	Article	IF	Citations
1	Mechanical properties of defective single-layered graphene sheets via molecular dynamics simulation. Superlattices and Microstructures, 2012, 51, 274-289.	1.4	158
2	Vibrations of single- and double-walled carbon nanotubes with layerwise boundary conditions: A molecular dynamics study. Current Applied Physics, 2012, 12, 707-711.	1.1	70
3	Fracture analysis of monolayer graphene sheets with double vacancy defects via MD simulation. Solid State Communications, 2011, 151, 1141-1146.	0.9	64
4	Mechanical properties of defective Î³-graphyne using molecular dynamics simulations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 561, 34-39.	2.6	59
5	Continuum and molecular dynamics study of C60 fullereneâ€“carbon nanotube oscillators. Mechanics Research Communications, 2013, 47, 18-23.	1.0	41
6	Structural and elastic properties and stability characteristics of oxygenated carbon nanotubes under physical adsorption of polymers. Applied Surface Science, 2015, 332, 640-647.	3.1	38
7	Elastic properties and large deformation of two-dimensional silicene nanosheets using molecular dynamics. Superlattices and Microstructures, 2014, 65, 64-70.	1.4	37
8	Elastic properties and buckling behavior of single-walled carbon nanotubes functionalized with diethyltoluenediamines using molecular dynamics simulations. Superlattices and Microstructures, 2015, 77, 54-63.	1.4	35
9	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, .	1.0	33
10	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.	1.2	33
11	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.	1.1	32
12	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.	1.9	29
13	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.	0.9	27
14	Vibration characteristics of single- and double-walled carbon nanotubes functionalized with amide and amine groups. Physica B: Condensed Matter, 2015, 462, 8-14.	1.3	27
15	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.	1.8	26
16	Torsional buckling behavior of boron-nitride nanotubes using molecular dynamics simulations. Current Applied Physics, 2014, 14, 1072-1077.	1.1	25
17	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.	3.1	25
18	Structural and elastic properties of hybrid bilayer graphene/h-BN with different interlayer distances using DFT. Superlattices and Microstructures, 2014, 72, 230-237.	1.4	23

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19	Vibrational characteristics of diethyltoluenediamines (DETDA) functionalized carbon nanotubes using molecular dynamics simulations. Physica B: Condensed Matter, 2015, 459, 58-61.	1.3	23
20	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.	3.1	23
21	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.	0.6	23
22	Molecular dynamics simulations of the polymer/amine functionalized single-walled carbon nanotubes interactions. Applied Surface Science, 2018, 455, 171-180.	3.1	21
23	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.	2.1	19
24	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.	1.9	19
25	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.	0.8	18
26	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.	1.1	17
27	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.	0.8	17
28	Interfacial characteristics and thermo-mechanical properties of calcium carbonate/polystyrene nanocomposite. Materials Chemistry and Physics, 2020, 247, 122871.	2.0	17
29	Oscillation characteristics of carbon nanotori molecules along carbon nanotubes under various system parameters. European Journal of Mechanics, A/Solids, 2017, 62, 67-79.	2.1	15
30	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.	1.3	14
31	Tensile characteristics of single-walled carbon nanotubes endohedrally decorated with gold nanowires: A molecular dynamics study. Diamond and Related Materials, 2019, 92, 117-129.	1.8	14
32	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.	1.7	14
33	Molecular dynamics investigation into the oscillatory behavior of double-walled boron-nitride nanotubes. Superlattices and Microstructures, 2016, 93, 18-26.	1.4	13
34	Structural and elastic properties of carbon nanotubes containing Fe atoms using first principles. Superlattices and Microstructures, 2013, 64, 220-226.	1.4	12
35	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.	0.8	12
36	Characterization of the mechanical properties of polyphenylene polymer using molecular dynamics simulations. Physica B: Condensed Matter, 2016, 481, 80-85.	1.3	12

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37	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.	1.3	12
38	Prediction of structural and mechanical properties of atom-decorated porous graphene via density functional calculations. EPJ Applied Physics, 2016, 74, 10401.	0.3	11
39	Tensile characteristics of carbene-functionalized CNTs subjected to physisorption of polymer chains: a molecular dynamics study. Journal of Molecular Modeling, 2019, 25, 318.	0.8	11
40	Investigation of the adsorption of polymer chains on amine-functionalized double-walled carbon nanotubes. Journal of Molecular Modeling, 2015, 21, 312.	0.8	10
41	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.	1.3	10
42	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.	0.7	10
43	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.	0.8	10
44	A molecular dynamics study on the buckling behavior of x-graphyne based single- and multi-walled nanotubes. Computational Materials Science, 2021, 191, 110333.	1.4	10
45	Continuum modeling of ion-selective membranes constructed from functionalized carbon nanotubes. European Physical Journal Plus, 2020, 135, 1.	1.2	9
46	On the Vibration of Single-Walled Carbon Nanocones: Molecular Mechanics Approach versus Molecular Dynamics Simulations. Shock and Vibration, 2014, 2014, 1-8.	0.3	8
47	On the Interfacial Properties of Polymers/Functionalized Single-Walled Carbon Nanotubes. Brazilian Journal of Physics, 2016, 46, 361-369.	0.7	8
48	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, 2021, 28, 2531-2550.	1.5	8
49	Influence of Electric Field on the Mechanical Properties of Hexagonal Boron-Nitride Sheets Using ab-initio Calculations. Nano, 2015, 10, 1550047.	0.5	7
50	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.	1.4	7
51	Stability analysis of endohedrally functionalized carbon nanotubes with pentagonal metallic nanowires: a molecular dynamics simulation approach. Materials Research Express, 2019, 6, 045056.	0.8	7
52	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.	2.1	7
53	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.	0.7	6
54	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.	0.6	6

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55	Characterization of the structural instability of BxCyNz heteronanotubes via molecular dynamics simulations. Materials Research Express, 2019, 6, 105096.	0.8	6
56	A molecular dynamics study on the buckling behavior of single-walled carbon nanotubes filled with gold nanowires. Journal of Molecular Modeling, 2020, 26, 196.	0.8	6
57	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.	0.9	6
58	Thermal conductivity of perfect and defective carbon nanotubes functionalized with carbene: a molecular dynamics study. Molecular Simulation, 0, , 1-9.	0.9	6
59	Mechanical properties and fracture analysis of defective penta-graphene under temperature variation: Insight from molecular dynamics. Diamond and Related Materials, 2022, 124, 108956.	1.8	6
60	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.	1.8	6
61	Characterization of the Mechanical Properties of Monolayer Molybdenum Disulfide Nanosheets Using First Principles. Journal of Nanotechnology in Engineering and Medicine, 2013, 4, .	0.8	5
62	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.	1.4	5
63	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.	1.4	5
64	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.	1.4	5
65	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.	0.8	4
66	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, 2021, 235, 5709-5717.	1.1	4
67	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.	0.6	3
68	Fundamental frequency analysis of endohedrally functionalized carbon nanotubes with metallic nanowires: a molecular dynamics study. Journal of Molecular Modeling, 2021, 27, 313.	0.8	3
69	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.	0.8	2
70	Structural stability and buckling analysis of a series of carbon nanotorus using molecular dynamics simulations. Journal of Molecular Modeling, 2018, 24, 263.	0.8	1
71	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.	1.0	1
72	Thermal conductivity of three-dimensional metallic carbon nanostructures (T6) with boron and nitrogen dopant. European Physical Journal D, 2020, 74, 1.	0.6	1

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73	Stacking Interactions of Poly Para-Phenylene Vinylene Oligomers with Graphene and Single-Walled Carbon Nanotubes: A Molecular Dynamics Approach. Molecules, 2020, 25, 4812.	1.7	1
74	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, 2022, 236, 3663-3671.	1.1	1
75	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.	1.0	0
76	High velocity impact analysis of free-free carbon nanotubes. Journal of Molecular Graphics and Modelling, 2022, 111, 108105.	1.3	0