Morteza Ghorbanzadeh Ahangari

List of Publications by Year in Descending Order

67 papers	1,325 citations	23 h-index	32 g-index
69 ext. papers	1,525 ext. citations	3.2 avg, IF	5.22 L-index

#	Paper	IF	Citations
67	Experiment and theory for acetylene adsorption in transformer oil. *Journal of Molecular Structure*, **2021**, 1230, 129860	3.4	0
66	Electronic, mechanical and thermal properties of SiO2 nanotube interacting with poly lactic-co-glycolic acid: Density functional theory and molecular dynamics studies. *Applied Surface Science*, **2021**, 546, 148894	6.7	4
65	H2 and H2S separation by adsorption using graphene and zinc oxide sheets: Molecular dynamic simulations. *Physica B: Condensed Matter*, **2021**, 619, 413175	2.8	1
64	Adsorption of hazardous atoms on the surface of TON zeolite and bilayer silica: a DFT study. *Journal of Molecular Modeling*, **2020**, 26, 119	2	6
63	Removal of methylmercaptan pollution using Ni and Pt-decorated graphene: an ab-initio DFT study. *Journal of Sulfur Chemistry*, **2020**, 41, 593-604	2.3	7
62	Experimental and multiscale quantum mechanics modeling of the mechanical properties of PVC/graphene nanocomposite. *Journal of Composite Materials*, **2020**, 54, 4575-4590	2.7	5
61	Density functional theory based molecular dynamics study on hydrogen storage capacity of C24, B12N12, Al12 N12, Be12O12, Mg12O12, and Zn12O12 nanocages. *International Journal of Hydrogen Energy*, **2020**, 45, 6745-6756	6.7	18
60	Density functional theory study on the interaction of chitosan monomer with TiO2, SiO2 and carbon nanotubes. *Materials Chemistry and Physics*, **2020**, 255, 123576	4.4	3
59	Effect of Nanosilica on the Mechanical and Thermal Properties of Carbon Fiber/Polycarbonate Laminates. *Fibers and Polymers*, **2019**, 20, 1684-1689	2	2
58	Alkane Cyclization: A DFT Study on the Effect of Chlorinated □Alumina. *Russian Journal of Physical Chemistry A*, **2019**, 93, 18-22	0.7	1
57	Effect of various defects on mechanical and electronic properties of zinc-oxide graphene-like structure: A DFT study. *Vacuum*, **2019**, 165, 26-34	3.7	34
56	Density Functional Theory Study on the Mechanical Properties and Interlayer Interactions of Multi-layer Graphene: Carbonic, Silicon-Carbide and Silicene Graphene-like Structures. *Silicon*, **2019**, 11, 1235-1246	2.4	25
55	The Effect of Interaction between Nanofillers and Epoxy on Mechanical and Thermal Properties of Nanocomposites: Theoretical Prediction and Experimental Analysis. *Advances in Polymer Technology*, **2019**, 2019, 1-10	1.9	17
54	Theoretical studies on the mechanical and electronic properties of 2D and 3D structures of Beryllium-Oxide graphene and graphene nanobud. *Applied Surface Science*, **2019**, 476, 36-48	6.7	32
53	Experimental study on the mechanical and thermal properties of basalt fiber and nanoclay reinforced polymer concrete. *Composite Structures*, **2018**, 191, 231-238	5.3	53
52	Computational studies at the density functional theory (DFT) level about the surface functionalization of hexagonal monolayers by chitosan monomer. *Applied Surface Science*, **2018**, 440, 778-789	6.7	10
51	Methane storage capacity of carbon fullerenes and their mechanical and electronic properties: Experimental and theoretical study. *Materials Chemistry and Physics*, **2018**, 211, 192-199	4.4	3

50	Pt/Au nanoalloy supported on alumina and chlorided alumina: DFT and experimental analysis. *Materials Research Express*, **2018**, 5, 045007	1.7	
49	Shape memory and mechanical properties of TPU/ABS blends: The role of pristine versus organo-modified carbon nanotubes. *Polymer Composites*, **2018**, 39, E984-E995	3	3
48	Mechanical properties of epoxy/basalt polymer concrete: Experimental and analytical study. *Structural Concrete*, **2018**, 19, 366-373	2.6	16
47	Effect of acrylonitrile butadiene styrene on the shape memory, mechanical, and thermal properties of thermoplastic polyurethane. *Journal of Vinyl and Additive Technology*, **2018**, 24, E96-E104	2	8
46	Density functional theory study of adsorption properties of non-carbon, carbon and functionalized graphene surfaces towards the zinc and lead atoms. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 104, 275-285	3	30
45	Atomistic Simulation of Mechanical Properties of Au32 Cluster Peapod Structures: Molecular Dynamics and Density Functional Theory. *Journal of Engineering Mechanics - ASCE*, **2018**, 144, 04018110	2.4	1
44	DFT study of Ni, Cu, Cd and Ag heavy metal atom adsorption onto the surface of the zinc-oxide nanotube and zinc-oxide graphene-like structure. *Materials Chemistry and Physics*, **2018**, 220, 366-373	4.4	47
43	Effect of basalt, silica sand and fly ash on the mechanical properties of quaternary polymer concretes. *Bulletin of Materials Science*, **2018**, 41, 1	1.7	9
42	DFT study of Au adsorption on pure and Pt-decorated □alumina (110) surface. *Applied Surface Science*, **2017**, 416, 390-396	6.7	13
41	Atomistic modeling of interfacial interaction between polyvinyl chloride and polypropylene with Boron-Nitride monolayer sheet: A density functional theory study. *Superlattices and Microstructures* , **2017**, 111, 23-31	2.8	26
40	Surface modification of carbon nanotubes using 3-aminopropyltriethoxysilane to improve mechanical properties of nanocomposite based polymer matrix: Experimental and Density functional theory study. *Applied Surface Science*, **2017**, 420, 167-179	6.7	31
39	Platinum adsorption onto graphene and oxidized graphene: A quantum mechanics study. *Materials Chemistry and Physics*, **2017**, 190, 17-24	4.4	5
38	Combining density functional theory-finite element multi-scale method to predict mechanical properties of polypropylene/graphene nanocomposites: Experimental study. *Materials Chemistry and Physics*, **2017**, 201, 214-223	4.4	29
37	Interlayer interaction and mechanical properties in multi-layer graphene, Boron-Nitride, Aluminum-Nitride and Gallium-Nitride graphene-like structure: A quantum-mechanical DFT study. *Superlattices and Microstructures*, **2017**, 112, 30-45	2.8	28
36	Investigation of heavy metal atoms adsorption onto graphene and graphdiyne surface: A density functional theory study. *Superlattices and Microstructures*, **2016**, 100, 1094-1102	2.8	51
35	The shape memory, and the mechanical and thermal properties of TPU/ABS/CNT: a ternary polymer composite. *RSC Advances*, **2016**, 6, 101038-101047	3.7	19
34	Interaction between fullerene-wheeled nanocar and gold substrate: A DFT study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2016**, 83, 174-179	3	11
33	Modeling of the interaction between polypropylene and monolayer sheets: a quantum mechanical study. *RSC Advances*, **2015**, 5, 80779-80785	3.7	18

32	Mechanical and electronic properties of carbon nanobuds: First-principles study. *Solid State Communications*, **2015**, 203, 58-62	1.6	15
31	Micromechanical properties and morphologies of self-healing epoxy nanocomposites with microencapsulated healing agent. *Materials Chemistry and Physics*, **2015**, 151, 112-118	4.4	24
30	Effect of defect and temperature on the mechanical and electronic properties of graphdiyne: A theoretical study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2015**, 66, 140-147	3	29
29	Epoxy monomer adsorption on Group III (B, Al, Ga) nitride nanotubes: vdW-DF studies on mechanical and electronic properties. *Superlattices and Microstructures*, **2014**, 67, 127-143	2.8	7
28	Density functional theory calculations of hydrogen molecule adsorption on monolayer molybdenum and tungsten disulfide. *Physica E: Low-Dimensional Systems and Nanostructures*, **2014**, 57, 28-34	3	13
27	Carborane-wheeled nanocar moving on graphene/graphyne surfaces: van der Waals corrected density functional theory study. *Materials Chemistry and Physics*, **2014**, 148, 435-443	4.4	24
26	First-principles vdW-DF study on the enhanced hydrogen storage capacity of Pt-adsorbed graphene. *Journal of Molecular Modeling*, **2014**, 20, 2230	2	14
25	Doping of carbon nanotubes with aluminum atom to improve Pt adsorption. *Applied Surface Science* , **2014**, 290, 86-91	6.7	16
24	Adsorption of H 2 S molecules on non-carbonic and decorated carbonic graphenes: A van der Waals density functional study. *Computational Materials Science*, **2014**, 92, 127-134	3.2	29
23	Effect of nanoparticles on the micromechanical and surface properties of poly(urea-formaldehyde) composite microcapsules. *Composites Part B: Engineering*, **2014**, 56, 450-455	10	59
22	Density functional theory study of epoxy polymer chains adsorbing onto single-walled carbon nanotubes: electronic and mechanical properties. *Journal of Molecular Modeling*, **2013**, 19, 3127-34	2	13
21	Si-decorated graphene: a superior media for lithium-ions storage. *Structural Chemistry*, **2013**, 24, 1473-1483	1.8	11
20	Electronic and mechanical properties of single-walled carbon nanotubes interacting with epoxy: A DFT study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2013**, 48, 148-156	3	34
19	Density functional theory based molecular dynamics simulation study on the bulk modulus of multi-shell fullerenes. *Physica B: Condensed Matter*, **2013**, 423, 1-5	2.8	10
18	Effect of nanoparticles on the morphology and thermal properties of self-healing poly(urea-formaldehyde) microcapsules. *Journal of Polymer Research*, **2013**, 20, 1	2.7	47
17	Pt-decorated graphene as superior media for H2S adsorption: A first-principles study. *Applied Surface Science*, **2012**, 261, 697-704	6.7	92
16	Effects of Nanoclay on Morphology, Rheological, and Mechanical Properties of Polyvinyl Chloride/Acrylonitrile-Butadiene-Styrene. *Polymer-Plastics Technology and Engineering*, **2012**, 51, 413-418		12
15	Elastic properties of SWCNTs with curved morphology: Density functional tight binding based treatment. *Solid State Communications*, **2012**, 152, 1526-1530	1.6	17

14	Density functional theory investigation of the mechanical properties of single-walled carbon nanotubes. *Computational Materials Science*, **2012**, 53, 377-381	3.2	29
13	Study of a Polymer Blend/Nanoclay Nanocomposite of Polyethylene and Polyamide 6 Prepared by Mechanical Blending. *Polymer-Plastics Technology and Engineering*, **2012**, 51, 80-85		15
12	Effect of Polypropylene Grafted Maleic Anhydride Compatibilizer on the Physical Properties of Polypropylene/Carbon Nanotube Composites. *Polymers and Polymer Composites*, **2012**, 20, 559-566	0.8	6
11	Investigation of the Mechanical Properties of Multi-Walled Carbon Nanotubes Using Density Functional Theory Calculations. *Journal of Computational and Theoretical Nanoscience*, **2012**, 9, 980-985	0.3	7
10	Study on Morphology, Rheology and Mechanical Properties of Thermoplastic Elastomer Polyolefin (TPO)/Carbon Nanotube Nanocomposites with Reference to the Effect of Polypropylene-grafted-Maleic Anhydride (PP-g-MA) as a Compatibilizer. *International Journal of Polymeric Materials and Polymeric Biomaterials*, **2011**, 60, 384-397	3	56
9	Effect of nano-nucleating agent addition on the isothermal and nonisothermal crystallization kinetics of isotactic polypropylene. *Polymer Bulletin*, **2011**, 66, 239-258	2.4	20
8	The Effect of Acid-Treatment of Carbon Nanotubes on the Thermal Kinetics of Isotactic Polypropylene. *Journal of Macromolecular Science - Physics*, **2011**, 50, 665-678	1.4	9
7	Damping Augmentation of Epoxy Using Carbon Nanotubes. *International Journal of Polymeric Materials and Polymeric Biomaterials*, **2010**, 60, 11-26	3	23
6	Effect of carbon nanotubes content on crystallization kinetics and morphology of polypropylene. *Polymer Testing*, **2009**, 28, 46-52	4.5	72
5	A DSC Study on the Nonisothermal Crystallization Kinetics of Polypropylene/Single-Walled Carbon Nanotube Nanocomposite. *Polymer-Plastics Technology and Engineering*, **2009**, 48, 579-586		23
4	Study of the Nonisothermal Crystallization Kinetics and Melting Behaviors of Polypropylene Reinforced with Single-Walled Carbon Nanotubes Nanocomposite. *Journal of Macromolecular Science - Physics*, **2009**, 48, 25-40	1.4	13
3	Thermal and Structural Behaviors of Polypropylene Nanocomposites Reinforced with Single-Walled Carbon Nanotubes by Melt Processing Method. *Journal of Macromolecular Science - Physics*, **2009**, 48, 196-211	1.4	18
2	Investigation of mechanical, thermal properties and non-isothermal crystallisation kinetic of polypropylene/single-walled carbon nanotube. *International Journal of Nano and Biomaterials*, **2009** , 2, 339	0.2	2
1	Mechanical properties of reinforced polymer concrete with three types of resin systems. *Proceedings of Institution of Civil Engineers: Construction Materials*,1-9	0.8	