Hamed Akbarzadeh

List of Publications by Year in Descending Order

106 papers	1,056 citations	17 h-index	23 g-index
108 ext. papers	1,211 ext. citations	4.4 avg, IF	5.02 L-index

#	Paper	IF	Citations
106	Concave Pd-M (M=Co, Ni, Cu, Rh, Ag, Ir, Pt, and Au) nanocubes explored by molecular dynamics simulations: A liquid-like expansion mechanism. *Applied Surface Science*, **2022**, 592, 153203	6.7	0
105	Investigation of doped carbon nanotubes on desalination process using molecular dynamics simulations. *Journal of Molecular Liquids*, **2021**, 348, 118040	6	2
104	Analysis of MoS2 and WS2 Nano-layers role on the radiation resistance of various Cu/MS2/Cu and Cu/MS2@Cu@MS2/Cu nanocomposites. *Materialia*, **2021**, 21, 101281	3.2	0
103	Pt core confined within an Au skeletal frame: Pt@Void@Au nanoframes in a molecular dynamics Perspective. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2021**, 631, 127664	5.1	1
102	Melting Behavior of Bimetallic and Trimetallic Nanoparticles: A Review of MD Simulation Studies. *Topics in Current Chemistry*, **2021**, 379, 22	7.2	2
101	Molecular dynamics simulation of carbon peapod-like nanomaterials in desalination process. *Desalination*, **2021**, 504, 114975	10.3	1
100	Stability of Pd@void@M (M=Ni, Ag, and Pt) yolk shell nanoparticles controlled by structural factors: A molecular dynamics perspective. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2021**, 610, 125920	5.1	0
99	Phase transitions in nanostructured water confined in carbon nanotubes by external electric and magnetic fields: a molecular dynamics investigation.. *RSC Advances*, **2021**, 11, 10532-10539	3.7	1
98	Structure, dynamics, and morphology of nanostructured water confined between parallel graphene surfaces and in carbon nanotubes by applying magnetic and electric fields. *Soft Matter*, **2021**, 17, 3085-3095	3.6	2
97	Investigation of the thermal properties of phase change materials encapsulated in capped carbon nanotubes using molecular dynamics simulations.. *RSC Advances*, **2021**, 11, 24594-24606	3.7	1
96	Thermodynamics, Structure, and Dynamic Properties of Nanostructured Water Confined into B-, N-, and Si-Doped Graphene Surfaces and Carbon Nanotubes. *Industrial & Engineering Chemistry Research*, **2020**, 59, 9642-9654	3.9	6
95	Molecular dynamics simulation of anticancer drug delivery from carbon nanotube using metal nanowires. *Journal of Computational Chemistry*, **2019**, 40, 2179-2190	3.5	2
94	AuIr nanoalloy nucleation during the gas-phase condensation: a comprehensive MD study including different effects. *Inorganic Chemistry Frontiers*, **2018**, 5, 1445-1457	6.8	12
93	Stability Control of Trimetallic Nanoparticles via AgPd Core Structure and Composition: A Molecular Dynamics Study. *Industrial & Engineering Chemistry Research*, **2018**, 57, 6236-6245	3.9	3
92	Unexpected trend for thermodynamic stability of Au@void@AgAu yolk-shell nanoparticles: A molecular dynamics study. *Applied Surface Science*, **2018**, 447, 648-655	6.7	3
91	Pt-Co nanocluster in hollow carbon nanospheres. *Journal of Computational Chemistry*, **2018**, 39, 1267-1274	3.5	4
90	Adsorption mechanism of different acyclovir concentrations on 12 nm sized magnetite nanoparticles: A molecular dynamics study. *Journal of Molecular Liquids*, **2018**, 254, 64-69	6	15

89	AgPd@Pt nanoparticles with different morphologies of cuboctahedron, icosahedron, decahedron, octahedron, and Marks-decahedron: insights from atomistic simulations. *Inorganic Chemistry Frontiers*, **2018**, 5, 870-878	6.8	12
88	Au□e nanoparticles visited by MD simulation: structural and thermodynamic properties affected by chemical composition. *New Journal of Chemistry*, **2018**, 42, 9666-9675	3.6	8
87	Formation of methane clathrates in carbon nanotubes: a molecular dynamics study. *New Journal of Chemistry*, **2018**, 42, 7083-7095	3.6	2
86	Rattle, Porous, and Dense Cores and Discontinuous Porous, Continuous Porous, and Dense Shells in [email□protected] Core□Shell Nanoparticles. *Industrial & Engineering Chemistry Research*, **2018**, 57, 4923-4934	3.9	1
85	Some properties of solid helium and helium nanoclusters using the effective HFD-like interaction potential: Adsorption and desorption inside carbon nanotube. *Physica A: Statistical Mechanics and Its Applications*, **2018**, 491, 219-232	3.3	1
84	Investigation of different effects on the capacity of supercapacitor comprising an ionic liquid between graphene oxide nanosheets. *Journal of Molecular Liquids*, **2018**, 266, 658-672	6	2
83	Ag□Au nanoparticles encapsulated inside porous hollow carbon nanospheres: a molecular dynamics study. *New Journal of Chemistry*, **2018**, 42, 13619-13628	3.6	5
82	Thermodynamic, structural, and dynamical properties of nano-confined water using SPC/E and TIP4P models by molecular dynamics simulations. *New Journal of Chemistry*, **2018**, 42, 16258-16272	3.6	7
81	Density-dependent phase transition in nano-confinement water using molecular dynamics simulation. *Journal of Molecular Liquids*, **2018**, 250, 26-34	6	7
80	Pt-Pd nanoalloys with crown-jewel structures: How size of the mother Pt cluster affects on thermal and structural properties of Pt-Pd nanoalloys?. *Journal of Molecular Liquids*, **2018**, 249, 477-485	6	8
79	Molecular dynamics simulation of liquid water and ice nanoclusters using a new effective HFD-like model. *Journal of Computational Chemistry*, **2018**, 39, 269-278	3.5	1
78	Effect of systematic addition of the third component on the melting characteristics and structural evolution of binary alloy nanoclusters. *Journal of Molecular Liquids*, **2018**, 249, 412-419	6	18
77	Investigation of Possible Formation of Au@M (M = Cu, Ir, Pt, and Rh) Core□Shell Nanoclusters in a Condensation□Coalescence Process Using Molecular Dynamics Simulations. *Industrial & Engineering Chemistry Research*, **2018**, 57, 14837-14845	3.9	12
76	Icosahedral Ir, Rh, Pt, and Cu nanoclusters into gold vapor environment: Thermodynamic and structural analysis of the formed core@shell nanoclusters using MD simulations. *Journal of Alloys and Compounds*, **2018**, 764, 323-332	5.7	11
75	Different morphologies of aluminum nanoclusters: Effect of pressure on solid-liquid phase transition of the nanoclusters using molecular dynamics simulations. *Journal of Molecular Liquids*, **2017**, 230, 20-23	6	10
74	Effect of pressure on some properties of Ag@Pd and Pd@Ag nanoclusters. *Journal of Alloys and Compounds*, **2017**, 703, 174-179	5.7	14
73	Ag-Au bimetallic nanoclusters formed from a homogeneous gas phase: a new thermodynamic expression confirmed by molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2017**, 19, 3763-3769	3.6	22
72	Competition between stability of icosahedral and cuboctahedral morphologies in bimetallic nanoalloys. *Physical Chemistry Chemical Physics*, **2017**, 19, 14659-14670	3.6	14

71	Au@Void@Ag Yolk-Shell Nanoclusters Visited by Molecular Dynamics Simulation: The Effects of Structural Factors on Thermodynamic Stability. *Journal of Physical Chemistry Letters*, **2017**, 8, 2990-2998	6.4	21
70	Investigation of solvation of iron nanoclusters in ionic liquid 1-butyl-1,1,1-trimethylammonium methane sulfonate using molecular dynamics simulations: Effect of cluster size at different temperatures. *Journal of Colloid and Interface Science*, **2017**, 504, 171-177	9.3	9
69	Thermal stabilities of iron nanoparticles under hydrostatic pressure. *Journal of Molecular Liquids*, **2017**, 241, 321-325	6	6
68	Delivery of Cisplatin Anti-Cancer Drug from Carbon, Boron Nitride, and Silicon Carbide Nanotubes Forced by Ag-Nanowire: A Comprehensive Molecular Dynamics Study. *Molecular Pharmaceutics*, **2017**, 14, 2273-2284	5.6	23
67	Dynamical investigation of formation of Ni Pt nanoclusters in gas phase. *Journal of Molecular Liquids*, **2017**, 240, 221-224	6	18
66	Kinetics formation of bimetallic nanoalloys at different simulation times. *Journal of Molecular Liquids*, **2017**, 240, 468-475	6	8
65	A comprehensive molecular dynamics investigation on confinement of Pt Cu nanocluster inside carbon nanotubes. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2017**, 522, 433-444	5.1	10
64	Au@void@AgAu Yolk-Shell Nanoparticles with Dominant Strain Effects: A Molecular Dynamics Simulation. *Journal of Physical Chemistry Letters*, **2017**, 8, 5064-5068	6.4	19
63	Ni-Co bimetallic nanoparticles with core-shell, alloyed, and Janus structures explored by MD simulation. *Journal of Molecular Liquids*, **2017**, 248, 1078-1095	6	14
62	Injection of mixture of shale gases in a nanoscale pore of graphite and their displacement by CO2/N2 gases using molecular dynamics study. *Journal of Molecular Liquids*, **2017**, 248, 439-446	6	11
61	Effect of support on the coalescence between Ag@Au nanoalloys using MD simulations. *Journal of Molecular Liquids*, **2017**, 244, 390-397	6	9
60	Au@Pt and Pt@Au nanoalloys in the icosahedral and cuboctahedral structures: Which is more stable?. *Journal of Molecular Liquids*, **2017**, 242, 1002-1017	6	10
59	Dumbbell-like, core–shell and Janus-like configurations in Pd@Au@Pd three-shell nanoalloys: a molecular dynamics study. *Inorganic Chemistry Frontiers*, **2017**, 4, 1551-1561	6.8	16
58	New molecular insights into the stability of Ni–Pd hollow nanoparticles. *Inorganic Chemistry Frontiers*, **2017**, 4, 1679-1690	6.8	13
57	Coalescence process of gold/silver core-shell nanoparticles located on carbon nanotube and graphene surfaces. *Journal of Molecular Liquids*, **2017**, 248, 738-750	6	6
56	Structural evolution of Pt/Pd nanoparticles in condensation process. *Journal of Molecular Liquids*, **2017**, 248, 822-829	6	11
55	Effects of pressure, nanoalloy size, and nanoalloy mole fraction on melting of Ir-Rh nanoalloys using molecular dynamics simulations. *Journal of Alloys and Compounds*, **2017**, 694, 1287-1294	5.7	15
54	Effect of Pt addition to Ag Au bimetallic nanoclusters: A molecular dynamics study of Ag Au Pt ternary system. *Journal of Alloys and Compounds*, **2017**, 692, 647-657	5.7	4

53	Mo nanocluster under high pressure: A molecular dynamics study. *Journal of Molecular Liquids*, **2016**, 222, 648-655	6	8
52	Phase transition in crown-jewel structured Au-Ir nanoalloys with different shapes: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2016**, 18, 25676-25686	3.6	16
51	A comprehensive study of methane/carbon dioxide adsorptive selectivity in different bundle nanotubes. *RSC Advances*, **2016**, 6, 69845-69854	3.7	4
50	Molecular dynamics simulation of noble gas adsorption on graphite: New effective potentials including many-body interactions. *Journal of Molecular Liquids*, **2016**, 222, 915-922	6	4
49	A molecular dynamics study of the effect of the substrate on the thermodynamic properties of bound Pt-Cu bimetallic nanoclusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 21730-6	3.6	8
48	Investigation of thermal, structural and dynamical properties of (AuxCuyNiy)N=32,108,256 ternary nanosystems: effect of Au addition to CuNi bimetallic nanoclusters via MD simulation. *RSC Advances*, **2016**, 6, 67619-67629	3.7	7
47	Au Pd nanoclusters supported on bundles of nanotubes and graphite surface: A comprehensive molecular dynamics study. *Journal of Alloys and Compounds*, **2016**, 687, 431-441	5.7	9
46	Adsorption of HeAr binary mixture on the silver nanoclusters: A molecular dynamics investigation on the effects mole fraction of mixture, shape and size of the nanocluster. *Journal of Molecular Liquids*, **2016**, 216, 111-116	6	5
45	Investigation of melting and freezing of AgAu alloy nanoclusters supported on carbon nanotube using molecular dynamics simulations. *Journal of Molecular Liquids*, **2016**, 216, 671-682	6	18
44	Nano-confined ionic liquid [emim][PF6] between graphite sheets: A molecular dynamics study. *Journal of Molecular Liquids*, **2016**, 215, 512-519	6	11
43	Carbon monoxide adsorption on the single-walled carbon nanotube supported goldsilver nanoalloys. *New Journal of Chemistry*, **2016**, 40, 310-319	3.6	9
42	Equation of state and some structural and dynamical properties of the confined Lennard-Jones fluid into carbon nanotube: A molecular dynamics study. *Physica A: Statistical Mechanics and Its Applications*, **2016**, 462, 1075-1090	3.3	2
41	A modified thermodynamic insight to deliquescence of a void-containing nanocrystal confirmed by MD simulation. *AICHE Journal*, **2016**, 62, 4066-4077	3.6	1
40	Propene adsorption on goldpalladium nanoalloys supported on bundle nanotubes. *RSC Advances*, **2016**, 6, 66275-66287	3.7	3
39	Investigation of size dependence of the properties of Cu nanoclusters using molecular dynamics simulations. *Journal of Molecular Liquids*, **2016**, 219, 158-164	6	9
38	Nanotube diameter dependency of anisotropic pressure of an ionic liquid confined in a carbon nanotube: A molecular dynamics study for [emim][PF6] case. *Journal of Molecular Liquids*, **2016**, 220, 370-374	6	2
37	Properties of silver nanoclusters and bulk silver, using a new and accurate HFD-like potential, including many-body interactions: the inversion scheme and molecular dynamics simulation. *RSC Advances*, **2016**, 6, 43924-43936	3.7	7
36	Melting behavior of (PdxPt1x)n nanoclusters confined in single-walled carbon nanotubes: a molecular dynamics investigation on the effects of chirality and diameter of nanotubes, and size and composition of nanoclusters. *RSC Advances*, **2015**, 5, 23160-23173	3.7	17

35	Molecular dynamics investigation on the deliquescence of NH4Cl and NH4NO3 nanoparticles under atmospheric conditions. *RSC Advances*, **2015**, 5, 38345-38353	3.7	3
34	Temperature and Doping Effect on Thermal Conductivity of Copper–Gold Icosahedral Bimetallic Nanoclusters and Bulk Structures. *Journal of Physical Chemistry C*, **2015**, 119, 7922-7932	3.8	12
33	Investigation of thermal evolution of copper nanoclusters encapsulated in carbon nanotubes: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2015**, 17, 12747-59	3.6	27
32	Investigation of thermodynamic, dynamic, and structural properties of H2 adsorption on a Ag-Au nanoalloy with a carbon nanotube support. *ChemPhysChem*, **2015**, 16, 1676-82	3.2	5
31	Investigation of the melting of ionic liquid [emim][PF6] confined inside carbon nanotubes using molecular dynamics simulations. *RSC Advances*, **2015**, 5, 3868-3874	3.7	27
30	Size dependence of the equation of state for Ne nanoclusters from an effective two-body potential via molecular dynamics simulations. *RSC Advances*, **2015**, 5, 11297-11308	3.7	15
29	Effects of diameter and chirality on structural and dynamical behavior of [EMIM][PF6] encapsulated in carbon nanotube: A molecular dynamics study. *Journal of Molecular Liquids*, **2015**, 212, 423-429	6	6
28	A new and accurate expression for the radial distribution function of confined Lennard-Jones fluid in carbon nanotubes. *RSC Advances*, **2015**, 5, 95781-95787	3.7	4
27	Disorder effect on heat capacity, self-diffusion coefficient, and choosing best potential model for melting temperature, in gold–copper bimetallic nanocluster with 55 atoms. *Journal of Nanoparticle Research*, **2015**, 17, 1	2.3	11
26	H2 adsorption on Ag-nanocluster/single-walled carbon nanotube composites: a molecular dynamics study on the effects of nanocluster size, diameter, and chirality of nanotube. *Journal of Computational Chemistry*, **2015**, 36, 433-40	3.5	20
25	Molecular dynamics simulations of silver nanocluster supported on carbon nanotube. *Journal of Colloid and Interface Science*, **2014**, 418, 178-84	9.3	47
24	Investigation of thermal behavior of graphite-supported Ag nanoclusters of different sizes using molecular dynamics simulations. *Fluid Phase Equilibria*, **2014**, 365, 68-73	2.5	11
23	A molecular dynamics investigation of hydrogen adsorption on Ag–Cu bimetallic nanoclusters supported on a bundle of single-walled carbon nanotubes. *RSC Advances*, **2014**, 4, 60866-60872	3.7	17
22	Accurate melting temperatures for Ne nanoclusters and bulk from an effective two-body potential via molecular dynamics simulations. *Fluid Phase Equilibria*, **2014**, 381, 90-94	2.5	4
21	Chemical ordering effect on melting temperature, surface energy of copper–gold bimetallic nanocluster. *Journal of Alloys and Compounds*, **2014**, 617, 746-750	5.7	24
20	Adsorption of He gas on the Agn nanoclusters: A molecular dynamic study. *Fluid Phase Equilibria*, **2014**, 379, 175-179	2.5	5
19	CO Adsorption on Ag Nanoclusters Supported on Carbon Nanotube: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2014**, 118, 9187-9195	3.8	49
18	Effects of Gas Adsorption on the Graphite-Supported Ag Nanoclusters: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2013**, 117, 26287-26294	3.8	35

17	Study of two dimensional anisotropic Ising models via a renormalization group approach. *Physica A: Statistical Mechanics and Its Applications*, **2013**, 392, 5604-5614	3.3	3
16	Cluster size dependence of surface energy of Ni nanoclusters: A molecular dynamics study. *Chemical Physics Letters*, **2013**, 558, 57-61	2.5	21
15	Permutation entropy and detrend fluctuation analysis for the natural complexity of cardiac heart interbeat signals. *Physica A: Statistical Mechanics and Its Applications*, **2013**, 392, 3106-3112	3.3	3
14	Intracellular viral infection kinetics using a stochastic approach. *Progress in Reaction Kinetics and Mechanism*, **2013**, 38, 359-376	0.5	
13	Dependence of self-diffusion coefficient, surface energy, on size, temperature, and Debye temperature on size for aluminum nanoclusters. *Fluid Phase Equilibria*, **2012**, 335, 26-31	2.5	17
12	Spin coupling and magnetic field effects on the finite-size free energy and its non-extensivity for 1-D Ising model with nearest and next-nearest neighbor interactions in nanosystem. *Phase Transitions*, **2012**, 85, 577-591	1.3	1
11	On the existence of an analytic solution to the 1-D Ising model with nearest and next-nearest neighbor interactions in the presence of a magnetic field. *Phase Transitions*, **2011**, 84, 77-84	1.3	4
10	Investigation of magnetic field effect on surface and finite-site free energy in one-dimensional Ising model of nanosystems. *Phase Transitions*, **2011**, 84, 613-623	1.3	1
9	Effect of water–ethanol content on the structure of Nafion in the sandwich model and solvent dynamics in nano-channels; a molecular dynamics study. *Molecular Physics*, **2011**, 109, 709-724	1.7	16
8	Denaturation of Drew-Dickerson DNA in a high salt concentration medium: molecular dynamics simulations. *Journal of Computational Chemistry*, **2011**, 32, 3354-61	3.5	9
7	Size dependence and effect of potential parameters on properties of nano-cavities in liquid xenon using molecular dynamics simulation. *Chemical Physics*, **2011**, 381, 44-48	2.3	2
6	Calculation of thermodynamic properties of Ni nanoclusters via selected equations of state based on molecular dynamics simulations. *Solid State Communications*, **2011**, 151, 965-970	1.6	25
5	Effect of a monomeric sequence on the structure of hydrated Nafion in the sandwich model and solvent dynamics in nano-channels: a molecular dynamic study. *Molecular Physics*, **2010**, 108, 3393-3404	1.7	2
4	Surface free energy of platinum nanoparticles at zero pressure: A molecular dynamic study. *Solid State Communications*, **2010**, 150, 254-257	1.6	12
3	Molecular dynamics simulation and MMPBSA calculations of sickle cell hemoglobin in dimer form with Val, Trp, or Phe at the lateral contact. *Journal of Physical Organic Chemistry*, **2010**, 23, 866-877	2.1	16
2	A molecular-dynamics study of thermal and physical properties of platinum nanoclusters. *Fluid Phase Equilibria*, **2009**, 280, 16-21	2.5	25
1	Using molecular dynamic simulation data of calcite in a wide pressure range to calculate some of its thermodynamic properties via some universal equations of state. *Molecular Physics*, **2008**, 106, 2545-2556	1.7	4