

# Hamed Akbarzadeh

## List of Publications by Citations

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106  
papers

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17  
h-index

23  
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108  
ext. papers

1,211  
ext. citations

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5.02  
L-index

#	Paper	IF	Citations
106	CO Adsorption on Ag Nanoclusters Supported on Carbon Nanotube: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 9187-9195	3.8	49
105	Molecular dynamics simulations of silver nanocluster supported on carbon nanotube. <i>Journal of Colloid and Interface Science</i> , <b>2014</b> , 418, 178-84	9.3	47
104	Effects of Gas Adsorption on the Graphite-Supported Ag Nanoclusters: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 26287-26294	3.8	35
103	Investigation of thermal evolution of copper nanoclusters encapsulated in carbon nanotubes: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 12747-59	3.6	27
102	Investigation of the melting of ionic liquid [emim][PF6] confined inside carbon nanotubes using molecular dynamics simulations. <i>RSC Advances</i> , <b>2015</b> , 5, 3868-3874	3.7	27
101	A molecular-dynamics study of thermal and physical properties of platinum nanoclusters. <i>Fluid Phase Equilibria</i> , <b>2009</b> , 280, 16-21	2.5	25
100	Calculation of thermodynamic properties of Ni nanoclusters via selected equations of state based on molecular dynamics simulations. <i>Solid State Communications</i> , <b>2011</b> , 151, 965-970	1.6	25
99	Chemical ordering effect on melting temperature, surface energy of copper-gold bimetallic nanocluster. <i>Journal of Alloys and Compounds</i> , <b>2014</b> , 617, 746-750	5.7	24
98	Delivery of Cisplatin Anti-Cancer Drug from Carbon, Boron Nitride, and Silicon Carbide Nanotubes Forced by Ag-Nanowire: A Comprehensive Molecular Dynamics Study. <i>Molecular Pharmaceutics</i> , <b>2017</b> , 14, 2273-2284	5.6	23
97	Ag-Au bimetallic nanoclusters formed from a homogeneous gas phase: a new thermodynamic expression confirmed by molecular dynamics simulation. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 3763-3769	3.6	22
96	Au@Void@Ag Yolk-Shell Nanoclusters Visited by Molecular Dynamics Simulation: The Effects of Structural Factors on Thermodynamic Stability. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 2990-2998	6.4	21
95	Cluster size dependence of surface energy of Ni nanoclusters: A molecular dynamics study. <i>Chemical Physics Letters</i> , <b>2013</b> , 558, 57-61	2.5	21
94	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. <i>Journal of Computational Chemistry</i> , <b>2015</b> , 36, 433-40	3.5	20
93	Au@void@AgAu Yolk-Shell Nanoparticles with Dominant Strain Effects: A Molecular Dynamics Simulation. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 5064-5068	6.4	19
92	Dynamical investigation of formation of Ni Pt nanoclusters in gas phase. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 240, 221-224	6	18
91	Investigation of melting and freezing of Ag-Au alloy nanoclusters supported on carbon nanotube using molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 216, 671-682	6	18
90	Effect of systematic addition of the third component on the melting characteristics and structural evolution of binary alloy nanoclusters. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 249, 412-419	6	18

89	Melting behavior of (PdxPt1-x) <sub>n</sub> 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. <i>RSC Advances</i> , <b>2015</b> , 5, 23160-23173	3.7	17
88	A molecular dynamics investigation of hydrogen adsorption on Ag <sub>10</sub> Au bimetallic nanoclusters supported on a bundle of single-walled carbon nanotubes. <i>RSC Advances</i> , <b>2014</b> , 4, 60866-60872	3.7	17
87	Dependence of self-diffusion coefficient, surface energy, on size, temperature, and Debye temperature on size for aluminum nanoclusters. <i>Fluid Phase Equilibria</i> , <b>2012</b> , 335, 26-31	2.5	17
86	Phase transition in crown-jewel structured Au-Ir nanoalloys with different shapes: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 25676-25686	3.6	16
85	Dumbbell-like, core-shell and Janus-like configurations in Pd@Au@Pd three-shell nanoalloys: a molecular dynamics study. <i>Inorganic Chemistry Frontiers</i> , <b>2017</b> , 4, 1551-1561	6.8	16
84	Effect of water/ethanol content on the structure of Nafion in the sandwich model and solvent dynamics in nano-channels; a molecular dynamics study. <i>Molecular Physics</i> , <b>2011</b> , 109, 709-724	1.7	16
83	Molecular dynamics simulation and MM/BSA calculations of sickle cell hemoglobin in dimer form with Val, Trp, or Phe at the lateral contact. <i>Journal of Physical Organic Chemistry</i> , <b>2010</b> , 23, 866-877	2.1	16
82	Adsorption mechanism of different acyclovir concentrations on 10 nm sized magnetite nanoparticles: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 254, 64-69	6	15
81	Effects of pressure, nanoalloy size, and nanoalloy mole fraction on melting of Ir-Rh nanoalloys using molecular dynamics simulations. <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 694, 1287-1294	5.7	15
80	Size dependence of the equation of state for Ne nanoclusters from an effective two-body potential via molecular dynamics simulations. <i>RSC Advances</i> , <b>2015</b> , 5, 11297-11308	3.7	15
79	Effect of pressure on some properties of Ag@Pd and Pd@Ag nanoclusters. <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 703, 174-179	5.7	14
78	Competition between stability of icosahedral and cuboctahedral morphologies in bimetallic nanoalloys. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 14659-14670	3.6	14
77	Ni-Co bimetallic nanoparticles with core-shell, alloyed, and Janus structures explored by MD simulation. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 248, 1078-1095	6	14
76	New molecular insights into the stability of Ni@Pd hollow nanoparticles. <i>Inorganic Chemistry Frontiers</i> , <b>2017</b> , 4, 1679-1690	6.8	13
75	Temperature and Doping Effect on Thermal Conductivity of Copper-Gold Icosahedral Bimetallic Nanoclusters and Bulk Structures. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 7922-7932	3.8	12
74	Au <sub>13</sub> nanoalloy nucleation during the gas-phase condensation: a comprehensive MD study including different effects. <i>Inorganic Chemistry Frontiers</i> , <b>2018</b> , 5, 1445-1457	6.8	12
73	AgPd@Pt nanoparticles with different morphologies of cuboctahedron, icosahedron, decahedron, octahedron, and Marks-decahedron: insights from atomistic simulations. <i>Inorganic Chemistry Frontiers</i> , <b>2018</b> , 5, 870-878	6.8	12
72	Surface free energy of platinum nanoparticles at zero pressure: A molecular dynamic study. <i>Solid State Communications</i> , <b>2010</b> , 150, 254-257	1.6	12

71	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. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2018</b> , 57, 14837-14845	3.9	12
70	Injection of mixture of shale gases in a nanoscale pore of graphite and their displacement by CO <sub>2</sub> /N <sub>2</sub> gases using molecular dynamics study. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 248, 439-446	6	11
69	Nano-confined ionic liquid [emim][PF <sub>6</sub> ] between graphite sheets: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 215, 512-519	6	11
68	Investigation of thermal behavior of graphite-supported Ag nanoclusters of different sizes using molecular dynamics simulations. <i>Fluid Phase Equilibria</i> , <b>2014</b> , 365, 68-73	2.5	11
67	Structural evolution of Pt/Pd nanoparticles in condensation process. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 248, 822-829	6	11
66	Disorder effect on heat capacity, self-diffusion coefficient, and choosing best potential model for melting temperature, in gold-copper bimetallic nanocluster with 55 atoms. <i>Journal of Nanoparticle Research</i> , <b>2015</b> , 17, 1	2.3	11
65	Icosahedral Ir, Rh, Pt, and Cu nanoclusters into gold vapor environment: Thermodynamic and structural analysis of the formed core@shell nanoclusters using MD simulations. <i>Journal of Alloys and Compounds</i> , <b>2018</b> , 764, 323-332	5.7	11
64	Different morphologies of aluminum nanoclusters: Effect of pressure on solid-liquid phase transition of the nanoclusters using molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 230, 20-23	6	10
63	A comprehensive molecular dynamics investigation on confinement of Pt Cu nanocluster inside carbon nanotubes. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , <b>2017</b> , 522, 433-444	5.1	10
62	Au@Pt and Pt@Au nanoalloys in the icosahedral and cuboctahedral structures: Which is more stable?. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 242, 1002-1017	6	10
61	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. <i>Journal of Colloid and Interface Science</i> , <b>2017</b> , 504, 171-177	9.3	9
60	Au Pd nanoclusters supported on bundles of nanotubes and graphite surface: A comprehensive molecular dynamics study. <i>Journal of Alloys and Compounds</i> , <b>2016</b> , 687, 431-441	5.7	9
59	Carbon monoxide adsorption on the single-walled carbon nanotube supported gold-silver nanoalloys. <i>New Journal of Chemistry</i> , <b>2016</b> , 40, 310-319	3.6	9
58	Effect of support on the coalescence between Ag@Au nanoalloys using MD simulations. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 244, 390-397	6	9
57	Denaturation of Drew-Dickerson DNA in a high salt concentration medium: molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , <b>2011</b> , 32, 3354-61	3.5	9
56	Investigation of size dependence of the properties of Cu nanoclusters using molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 219, 158-164	6	9
55	Kinetics formation of bimetallic nanoalloys at different simulation times. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 240, 468-475	6	8
54	AuBe nanoparticles visited by MD simulation: structural and thermodynamic properties affected by chemical composition. <i>New Journal of Chemistry</i> , <b>2018</b> , 42, 9666-9675	3.6	8

53	Mo nanocluster under high pressure: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 222, 648-655	6	8
52	A molecular dynamics study of the effect of the substrate on the thermodynamic properties of bound Pt-Cu bimetallic nanoclusters. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 21730-6	3.6	8
51	Pt-Pd nanoalloys with crown-jewel structures: How size of the mother Pt cluster affects on thermal and structural properties of Pt-Pd nanoalloys?. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 249, 477-485	6	8
50	Investigation of thermal, structural and dynamical properties of (Au <sub>12</sub> Cu <sub>12</sub> ) <sub>N</sub> =32,108,256 ternary nanosystems: effect of Au addition to Cu <sub>12</sub> bimetallic nanoclusters via MD simulation. <i>RSC Advances</i> , <b>2016</b> , 6, 67619-67629	3.7	7
49	Thermodynamic, structural, and dynamical properties of nano-confined water using SPC/E and TIP4P models by molecular dynamics simulations. <i>New Journal of Chemistry</i> , <b>2018</b> , 42, 16258-16272	3.6	7
48	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. <i>RSC Advances</i> , <b>2016</b> , 6, 43924-43936	3.7	7
47	Density-dependent phase transition in nano-confinement water using molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 250, 26-34	6	7
46	Thermal stabilities of iron nanoparticles under hydrostatic pressure. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 241, 321-325	6	6
45	Thermodynamics, Structure, and Dynamic Properties of Nanostructured Water Confined into B-, N-, and Si-Doped Graphene Surfaces and Carbon Nanotubes. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2020</b> , 59, 9642-9654	3.9	6
44	Coalescence process of gold/silver core-shell nanoparticles located on carbon nanotube and graphene surfaces. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 248, 738-750	6	6
43	Effects of diameter and chirality on structural and dynamical behavior of [EMIM][PF6] encapsulated in carbon nanotube: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , <b>2015</b> , 212, 423-429	6	6
42	Investigation of thermodynamic, dynamic, and structural properties of H <sub>2</sub> adsorption on a Ag-Au nanoalloy with a carbon nanotube support. <i>ChemPhysChem</i> , <b>2015</b> , 16, 1676-82	3.2	5
41	Adsorption of He/Ar binary mixture on the silver nanoclusters: A molecular dynamics investigation on the effects mole fraction of mixture, shape and size of the nanocluster. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 216, 111-116	6	5
40	Ag/Au nanoparticles encapsulated inside porous hollow carbon nanospheres: a molecular dynamics study. <i>New Journal of Chemistry</i> , <b>2018</b> , 42, 13619-13628	3.6	5
39	Adsorption of He gas on the Ag <sub>n</sub> nanoclusters: A molecular dynamic study. <i>Fluid Phase Equilibria</i> , <b>2014</b> , 379, 175-179	2.5	5
38	Pt-Co nanocluster in hollow carbon nanospheres. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 1267-1274	3.5	4
37	A comprehensive study of methane/carbon dioxide adsorptive selectivity in different bundle nanotubes. <i>RSC Advances</i> , <b>2016</b> , 6, 69845-69854	3.7	4
36	Molecular dynamics simulation of noble gas adsorption on graphite: New effective potentials including many-body interactions. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 222, 915-922	6	4

35	Accurate melting temperatures for Ne nanoclusters and bulk from an effective two-body potential via molecular dynamics simulations. <i>Fluid Phase Equilibria</i> , <b>2014</b> , 381, 90-94	2.5	4
34	Effect of Pt addition to Ag Au bimetallic nanoclusters: A molecular dynamics study of Ag Au Pt ternary system. <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 692, 647-657	5.7	4
33	A new and accurate expression for the radial distribution function of confined Lennard-Jones fluid in carbon nanotubes. <i>RSC Advances</i> , <b>2015</b> , 5, 95781-95787	3.7	4
32	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. <i>Phase Transitions</i> , <b>2011</b> , 84, 77-84	1.3	4
31	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. <i>Molecular Physics</i> , <b>2008</b> , 106, 2545-2556	1.7	4
30	Molecular dynamics investigation on the deliquescence of NH <sub>4</sub> Cl and NH <sub>4</sub> NO <sub>3</sub> nanoparticles under atmospheric conditions. <i>RSC Advances</i> , <b>2015</b> , 5, 38345-38353	3.7	3
29	Stability Control of [email protected] Trimetallic Nanoparticles via AgPd Core Structure and Composition: A Molecular Dynamics Study. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2018</b> , 57, 6236-6245	3.9	3
28	Unexpected trend for thermodynamic stability of Au@void@AgAu yolk-shell nanoparticles: A molecular dynamics study. <i>Applied Surface Science</i> , <b>2018</b> , 447, 648-655	6.7	3
27	Study of two dimensional anisotropic Ising models via a renormalization group approach. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2013</b> , 392, 5604-5614	3.3	3
26	Permutation entropy and detrend fluctuation analysis for the natural complexity of cardiac heart interbeat signals. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2013</b> , 392, 3106-3112	3.3	3
25	Propene adsorption on gold-palladium nanoalloys supported on bundle nanotubes. <i>RSC Advances</i> , <b>2016</b> , 6, 66275-66287	3.7	3
24	Molecular dynamics simulation of anticancer drug delivery from carbon nanotube using metal nanowires. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 2179-2190	3.5	2
23	Formation of methane clathrates in carbon nanotubes: a molecular dynamics study. <i>New Journal of Chemistry</i> , <b>2018</b> , 42, 7083-7095	3.6	2
22	Investigation of different effects on the capacity of supercapacitor comprising an ionic liquid between graphene oxide nanosheets. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 266, 658-672	6	2
21	Size dependence and effect of potential parameters on properties of nano-cavities in liquid xenon using molecular dynamics simulation. <i>Chemical Physics</i> , <b>2011</b> , 381, 44-48	2.3	2
20	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. <i>Molecular Physics</i> , <b>2010</b> , 108, 3393-3404	1.7	2
19	Investigation of doped carbon nanotubes on desalination process using molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 348, 118040	6	2
18	Melting Behavior of Bimetallic and Trimetallic Nanoparticles: A Review of MD Simulation Studies. <i>Topics in Current Chemistry</i> , <b>2021</b> , 379, 22	7.2	2

17	Equation of state and some structural and dynamical properties of the confined Lennard-Jones fluid into carbon nanotube: A molecular dynamics study. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2016</b> , 462, 1075-1090	3.3	2
16	Nanotube diameter dependency of anisotropic pressure of an ionic liquid confined in a carbon nanotube: A molecular dynamics study for [emim][PF6] case. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 220, 370-374	6	2
15	Structure, dynamics, and morphology of nanostructured water confined between parallel graphene surfaces and in carbon nanotubes by applying magnetic and electric fields. <i>Soft Matter</i> , <b>2021</b> , 17, 3085-3095	3.6	2
14	Rattle, Porous, and Dense Cores and Discontinuous Porous, Continuous Porous, and Dense Shells in [email protected] Core/Shell Nanoparticles. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2018</b> , 57, 4923-4934	3.9	1
13	Some properties of solid helium and helium nanoclusters using the effective HFD-like interaction potential: Adsorption and desorption inside carbon nanotube. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2018</b> , 491, 219-232	3.3	1
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. <i>Phase Transitions</i> , <b>2012</b> , 85, 577-591	1.3	1
11	Investigation of magnetic field effect on surface and finite-site free energy in one-dimensional Ising model of nanosystems. <i>Phase Transitions</i> , <b>2011</b> , 84, 613-623	1.3	1
10	Pt core confined within an Au skeletal frame: Pt@Void@Au nanoframes in a molecular dynamics Perspective. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , <b>2021</b> , 631, 127664	5.1	1
9	Molecular dynamics simulation of carbon peapod-like nanomaterials in desalination process. <i>Desalination</i> , <b>2021</b> , 504, 114975	10.3	1
8	A modified thermodynamic insight to deliquescence of a void-containing nanocrystal confirmed by MD simulation. <i>AIChE Journal</i> , <b>2016</b> , 62, 4066-4077	3.6	1
7	Phase transitions in nanostructured water confined in carbon nanotubes by external electric and magnetic fields: a molecular dynamics investigation.. <i>RSC Advances</i> , <b>2021</b> , 11, 10532-10539	3.7	1
6	Molecular dynamics simulation of liquid water and ice nanoclusters using a new effective HFD-like model. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 269-278	3.5	1
5	Investigation of the thermal properties of phase change materials encapsulated in capped carbon nanotubes using molecular dynamics simulations.. <i>RSC Advances</i> , <b>2021</b> , 11, 24594-24606	3.7	1
4	Analysis of MoS2 and WS2 Nano-layers role on the radiation resistance of various Cu/MS2/Cu and Cu/MS2@Cu@MS2/Cu nanocomposites. <i>Materialia</i> , <b>2021</b> , 21, 101281	3.2	0
3	Stability of Pd@void@M (M=Ni, Ag, and Pt) yolk shell nanoparticles controlled by structural factors: A molecular dynamics perspective. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , <b>2021</b> , 610, 125920	5.1	0
2	Concave Pd-M (M=Co, Ni, Cu, Rh, Ag, Ir, Pt, and Au) nanocubes explored by molecular dynamics simulations: A liquid-like expansion mechanism. <i>Applied Surface Science</i> , <b>2022</b> , 592, 153203	6.7	0
1	Intracellular viral infection kinetics using a stochastic approach. <i>Progress in Reaction Kinetics and Mechanism</i> , <b>2013</b> , 38, 359-376	0.5	