Hamed Akbarzadeh

List of Publications by Year
in descending order

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108	1,346	394286 19	526166 27
papers	citations	h-index	g-index

108	108	108	848
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CO Adsorption on Ag Nanoclusters Supported on Carbon Nanotube: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2014, 118, 9187-9195.	1.5	53
2	Molecular dynamics simulations of silver nanocluster supported on carbon nanotube. Journal of Colloid and Interface Science, 2014, 418, 178-184.	5.0	49
3	Effects of Gas Adsorption on the Graphite-Supported Ag Nanoclusters: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2013, 117, 26287-26294.	1.5	40
4	Investigation of the melting of ionic liquid [emim][PF₆] confined inside carbon nanotubes using molecular dynamics simulations. RSC Advances, 2015, 5, 3868-3874.	1.7	31
5	Chemical ordering effect on melting temperature, surface energy of copperâ€“gold bimetallic nanocluster. Journal of Alloys and Compounds, 2014, 617, 746-750.	2.8	29
6	Investigation of thermal evolution of copper nanoclusters encapsulated in carbon nanotubes: a molecular dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 12747-12759.	1.3	29
7	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.	2.3	29
8	A molecular-dynamics study of thermal and physical properties of platinum nanoclusters. Fluid Phase Equilibria, 2009, 280, 16-21.	1.4	27
9	Au@Void@Ag Yolkâ€“Shell Nanoclusters Visited by Molecular Dynamics Simulation: The Effects of Structural Factors on Thermodynamic Stability. Journal of Physical Chemistry Letters, 2017, 8, 2990-2998.	2.1	27
10	Adsorption mechanism of different acyclovir concentrations on 1â€“2â€¯nm sized magnetite nanoparticles: A molecular dynamics study. Journal of Molecular Liquids, 2018, 254, 64-69.	2.3	26
11	Calculation of thermodynamic properties of Ni nanoclusters via selected equations of state based on molecular dynamics simulations. Solid State Communications, 2011, 151, 965-970.	0.9	25
12	Agâ€“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.	1.3	24
13	Au@void@AgAu Yolkâ€“Shell Nanoparticles with Dominant Strain Effects: A Molecular Dynamics Simulation. Journal of Physical Chemistry Letters, 2017, 8, 5064-5068.	2.1	24
14	Investigation of doped carbon nanotubes on desalination process using molecular dynamics simulations. Journal of Molecular Liquids, 2022, 348, 118040.	2.3	24
15	Molecular dynamics simulation and MMâ€“PBSA 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.	0.9	23
16	Ni-Co bimetallic nanoparticles with core-shell, alloyed, and Janus structures explored by MD simulation. Journal of Molecular Liquids, 2017, 248, 1078-1095.	2.3	23
17	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.	2.3	23
18	Cluster size dependence of surface energy of Ni nanoclusters: A molecular dynamics study. Chemical Physics Letters, 2013, 558, 57-61.	1.2	21

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19	H₂adsorption 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, 433-440.	1.5	21
20	Investigation of melting and freezing of Agâ€“Au alloy nanoclusters supported on carbon nanotube using molecular dynamics simulations. Journal of Molecular Liquids, 2016, 216, 671-682.	2.3	21
21	Molecular dynamics simulation of carbon peapod-like nanomaterials in desalination process. Desalination, 2021, 504, 114975.	4.0	21
22	Phase transition in crown-jewel structured Auâ€“Ir nanoalloys with different shapes: a molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 25676-25686.	1.3	20
23	A molecular dynamics investigation of hydrogen adsorption on Agâ€“Cu bimetallic nanoclusters supported on a bundle of single-walled carbon nanotubes. RSC Advances, 2014, 4, 60866-60872.	1.7	19
24	Melting behavior of (Pd_xPt_{1â^'x})_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.	1.7	19
25	Dynamical investigation of formation of Ni Pt nanoclusters in gas phase. Journal of Molecular Liquids, 2017, 240, 221-224.	2.3	19
26	Dumbbell-like, coreâ€“shell and Janus-like configurations in Pd@Au@Pd three-shell nanoalloys: a molecular dynamics study. Inorganic Chemistry Frontiers, 2017, 4, 1551-1561.	3.0	19
27	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.	1.4	18
28	New molecular insights into the stability of Niâ€“Pd hollow nanoparticles. Inorganic Chemistry Frontiers, 2017, 4, 1679-1690.	3.0	18
29	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.	3.0	18
30	Effect of waterâ€“methanol 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.	0.8	17
31	Effect of pressure on some properties of Ag@Pd and Pd@Ag nanoclusters. Journal of Alloys and Compounds, 2017, 703, 174-179.	2.8	17
32	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.	1.7	16
33	Competition between stability of icosahedral and cuboctahedral morphologies in bimetallic nanoalloys. Physical Chemistry Chemical Physics, 2017, 19, 14659-14670.	1.3	16
34	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.	2.8	16
35	Melting Behavior of Bimetallic and Trimetallic Nanoparticles: A Review of MD Simulation Studies. Topics in Current Chemistry, 2021, 379, 22.	3.0	15
36	Temperature and Doping Effect on Thermal Conductivity of Copperâ€“Gold Icosahedral Bimetallic Nanoclusters and Bulk Structures. Journal of Physical Chemistry C, 2015, 119, 7922-7932.	1.5	14

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37	Nano-confined ionic liquid [emim][PF6] between graphite sheets: A molecular dynamics study. Journal of Molecular Liquids, 2016, 215, 512-519.	2.3	14
38	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.	2.3	14
39	Auâ€“Ir nanoalloy nucleation during the gas-phase condensation: a comprehensive MD study including different effects. Inorganic Chemistry Frontiers, 2018, 5, 1445-1457.	3.0	14
40	Investigation of the thermal properties of phase change materials encapsulated in capped carbon nanotubes using molecular dynamics simulations. RSC Advances, 2021, 11, 24594-24606.	1.7	14
41	Surface free energy of platinum nanoparticles at zero pressure: A molecular dynamic study. Solid State Communications, 2010, 150, 254-257.	0.9	13
42	Investigation of thermal behavior of graphite-supported Ag nanoclusters of different sizes using molecular dynamics simulations. Fluid Phase Equilibria, 2014, 365, 68-73.	1.4	13
43	Disorder effect on heat capacity, self-diffusion coefficient, and choosing best potential model for melting temperature, in goldâ€“copper bimetallic nanocluster with 55 atoms. Journal of Nanoparticle Research, 2015, 17, 1.	0.8	13
44	Investigation of Possible Formation of Au@M (M = Cu, Ir, Pt, and Rh) Coreâ€“Shell Nanoclusters in a Condensationâ€“Coalescence Process Using Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2018, 57, 14837-14845.	1.8	13
45	Carbon monoxide adsorption on the single-walled carbon nanotube supported goldâ€“silver nanoalloys. New Journal of Chemistry, 2016, 40, 310-319.	1.4	12
46	Au@Pt and Pt@Au nanoalloys in the icosahedral and cuboctahedral structures: Which is more stable?. Journal of Molecular Liquids, 2017, 242, 1002-1017.	2.3	12
47	Structural evolution of Pt/Pd nanoparticles in condensation process. Journal of Molecular Liquids, 2017, 248, 822-829.	2.3	12
48	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.	2.3	11
49	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.	2.8	11
50	Denaturation of Drewâ€“Dickerson DNA in a high salt concentration medium: Molecular dynamics simulations. Journal of Computational Chemistry, 2011, 32, 3354-3361.	1.5	10
51	A molecular dynamics study of the effect of the substrate on the thermodynamic properties of bound Ptâ€“Cu bimetallic nanoclusters. Physical Chemistry Chemical Physics, 2016, 18, 21730-21736.	1.3	10
52	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.	2.8	10
53	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.	2.3	10
54	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.	5.0	10

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55	Kinetics formation of bimetallic nanoalloys at different simulation times. Journal of Molecular Liquids, 2017, 240, 468-475.	2.3	10
56	Effect of support on the coalescence between Ag@Au nanoalloys using MD simulations. Journal of Molecular Liquids, 2017, 244, 390-397.	2.3	10
57	Investigation of size dependence of the properties of Cu nanoclusters using molecular dynamics simulations. Journal of Molecular Liquids, 2016, 219, 158-164.	2.3	9
58	Stability Control of AgPd@Pt Trimetallic Nanoparticles via Agâ€“Pd Core Structure and Composition: A Molecular Dynamics Study. Industrial & Engineering Chemistry Research, 2018, 57, 6236-6245.	1.8	9
59	Auâ€“Fe nanoparticles visited by MD simulation: structural and thermodynamic properties affected by chemical composition. New Journal of Chemistry, 2018, 42, 9666-9675.	1.4	9
60	Density-dependent phase transition in nano-confinement water using molecular dynamics simulation. Journal of Molecular Liquids, 2018, 250, 26-34.	2.3	9
61	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.	2.3	9
62	Agâ€“Au nanoparticles encapsulated inside porous hollow carbon nanospheres: a molecular dynamics study. New Journal of Chemistry, 2018, 42, 13619-13628.	1.4	9
63	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.	1.4	9
64	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.	1.8	9
65	Mo nanocluster under high pressure: A molecular dynamics study. Journal of Molecular Liquids, 2016, 222, 648-655.	2.3	8
66	Investigation of thermal, structural and dynamical properties of (Au_xâ€“Cu_yâ€“Ni_y)_{N=32,108,256} ternary nanosystems: effect of Au addition to Cuâ€“Ni bimetallic nanoclusters via MD simulation. RSC Advances, 2016, 6, 67619-67629.	1.7	8
67	Molecular dynamics simulation of anticancer drug delivery from carbon nanotube using metal nanowires. Journal of Computational Chemistry, 2019, 40, 2179-2190.	1.5	8
68	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.	2.3	7
69	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.	1.7	7
70	A comprehensive study of methane/carbon dioxide adsorptive selectivity in different bundle nanotubes. RSC Advances, 2016, 6, 69845-69854.	1.7	7
71	Molecular dynamics simulation of noble gas adsorption on graphite: New effective potentials including many-body interactions. Journal of Molecular Liquids, 2016, 222, 915-922.	2.3	7
72	Unexpected trend for thermodynamic stability of Au@void@AgAu yolk-shell nanoparticles: A molecular dynamics study. Applied Surface Science, 2018, 447, 648-655.	3.1	7

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73	Ptâ€“Co nanocluster in hollow carbon nanospheres. Journal of Computational Chemistry, 2018, 39, 1267-1274.	1.5	7
74	A new and accurate expression for the radial distribution function of confined Lennard-Jones fluid in carbon nanotubes. RSC Advances, 2015, 5, 95781-95787.	1.7	6
75	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.	1.2	6
76	Thermal stabilities of iron nanoparticles under hydrostatic pressure. Journal of Molecular Liquids, 2017, 241, 321-325.	2.3	6
77	Coalescence process of gold/silver core-shell nanoparticles located on carbon nanotube and graphene surfaces. Journal of Molecular Liquids, 2017, 248, 738-750.	2.3	6
78	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.	2.8	6
79	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, 2022, 21, 101281.	1.3	6
80	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.	0.6	5
81	Adsorption of He gas on the Agn nanoclusters: A molecular dynamic study. Fluid Phase Equilibria, 2014, 379, 175-179.	1.4	5
82	Investigation of Thermodynamic, Dynamic, and Structural Properties of H₂ Adsorption on a Agâ€“Au Nanoalloy with a Carbon Nanotube Support. ChemPhysChem, 2015, 16, 1676-1682.	1.0	5
83	Adsorption of Heâ€“Ar 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.	2.3	5
84	Formation of methane clathrates in carbon nanotubes: a molecular dynamics study. New Journal of Chemistry, 2018, 42, 7083-7095.	1.4	5
85	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.	0.8	4
86	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.	1.2	4
87	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.	1.4	4
88	Rattle, Porous, and Dense Cores and Discontinuous Porous, Continuous Porous, and Dense Shells in Pt@Au Coreâ€“Shell Nanoparticles. Industrial & Engineering Chemistry Research, 2018, 57, 4923-4934.	1.8	4
89	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.	2.3	4
90	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.	2.3	4

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91	Study of two dimensional anisotropic Ising models via a renormalization group approach. Physica A: Statistical Mechanics and Its Applications, 2013, 392, 5604-5614.	1.2	3
92	Molecular dynamics investigation on the deliquescence of NH₄Cl and NH₄NO₃nanoparticles under atmospheric conditions. RSC Advances, 2015, 5, 38345-38353.	1.7	3
93	Propene adsorption on goldâ€“palladium nanoalloys supported on bundle nanotubes. RSC Advances, 2016, 6, 66275-66287.	1.7	3
94	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.	2.3	3
95	Concave Pd-M (MÂ=ÂCo, 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.	3.1	3
96	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.	0.8	2
97	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.	0.9	2
98	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.	1.2	2
99	Molecular dynamics simulation of liquid water and ice nanoclusters using a new effective HFDâ€like model. Journal of Computational Chemistry, 2018, 39, 269-278.	1.5	2
100	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.	1.7	2
101	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.	1.2	2
102	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.	2.3	2
103	Boron Nitride- and Graphene-Supported Trimetallic Yolkâ€“Shell and Hollow Nanoparticles. Industrial & Engineering Chemistry Research, 0, , .	1.8	2
104	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.	0.6	1
105	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.	0.6	1
106	Intracellular viral infection kinetics using a stochastic approach. Progress in Reaction Kinetics and Mechanism, 2013, 38, 359-376.	1.1	1
107	A modified thermodynamic insight to deliquescence of a voidâ€containing nanocrystal confirmed by MD simulation. AICHE Journal, 2016, 62, 4066-4077.	1.8	1
108	Ball-Cup, Janus, core-shell and disordered-alloy rhodium-gold nanoparticles: An atomistic simulation on structural stability. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 651, 129658.	2.3	1