Mohsen Abbaspour

List of Publications by Year
in descending order

67	773	516561 16	677027 22
papers	citations	h-index	g-index

67	67	67	497
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An accurate expression for radial distribution function of the Lennard-Jones fluid. Chemical Physics, 2005, 310, 11-15.	0.9	44
2	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
3	Molecular Dynamics Simulation of Argon, Krypton, and Xenon Using Two-Body and Three-Body Intermolecular Potentials. Journal of Chemical Theory and Computation, 2006, 2, 920-926.	2.3	30
4	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
5	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
6	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
7	Investigation of doped carbon nanotubes on desalination process using molecular dynamics simulations. Journal of Molecular Liquids, 2022, 348, 118040.	2.3	24
8	Computation of some thermodynamics, transport, structural properties, and new equation of state for fluid neon using a new intermolecular potential from molecular dynamics simulation. Theoretical Chemistry Accounts, 2010, 127, 573-585.	0.5	22
9	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
10	Molecular dynamics simulation of carbon peapod-like nanomaterials in desalination process. Desalination, 2021, 504, 114975.	4.0	21
11	Quantum computation of the properties of helium using two-body and three-body intermolecular potentials: a molecular dynamics study. Theoretical Chemistry Accounts, 2008, 119, 355-368.	0.5	20
12	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
13	Dynamical investigation of formation of Ni Pt nanoclusters in gas phase. Journal of Molecular Liquids, 2017, 240, 221-224.	2.3	19
14	New molecular insights into the stability of Niâ€“Pd hollow nanoparticles. Inorganic Chemistry Frontiers, 2017, 4, 1679-1690.	3.0	18
15	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
16	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
17	Melting Behavior of Bimetallic and Trimetallic Nanoparticles: A Review of MD Simulation Studies. Topics in Current Chemistry, 2021, 379, 22.	3.0	15
18	Determination of potential energy functions of COâ€“CO, CO2â€“CO2, and N2Oâ€“N2O and calculation of their transport properties. Chemical Physics, 2006, 330, 313-325.	0.9	14

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19	Transport, thermodynamic, and structural properties of fluid ammonia using a new intermolecular potential: The inversion method and molecular dynamics simulation. Chemical Physics, 2011, 389, 121-127.	0.9	14
20	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
21	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
22	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
23	Determination of potential energy function of methane via the inversion of reduced viscosity collision integrals at zero pressure. Fluid Phase Equilibria, 2003, 212, 53-65.	1.4	12
24	Determination of potential energy functions and calculation transport properties of oxygen and nitric oxide via the inversion of reduced viscosity collision integrals at zero pressure. Chemical Physics, 2006, 326, 620-630.	0.9	12
25	Carbon monoxide adsorption on the single-walled carbon nanotube supported goldâ€“silver nanoalloys. New Journal of Chemistry, 2016, 40, 310-319.	1.4	12
26	Structural evolution of Pt/Pd nanoparticles in condensation process. Journal of Molecular Liquids, 2017, 248, 822-829.	2.3	12
27	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
28	Ag, Au, Pt, and Au-Pt nanoclusters in [N1114][C1SO3] ionic liquid: A molecular dynamics study. Journal of Molecular Liquids, 2022, 360, 119447.	2.3	11
29	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
30	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
31	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
32	Determination of the Potential Energy Function of CF4â^'CF4via the Inversion of Reduced Viscosity Collision Integrals at Zero Pressure. Industrial & Engineering Chemistry Research, 2003, 42, 2256-2261.	1.8	9
33	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
34	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
35	Density-dependent phase transition in nano-confinement water using molecular dynamics simulation. Journal of Molecular Liquids, 2018, 250, 26-34.	2.3	9
36	Agâ€“Au nanoparticles encapsulated inside porous hollow carbon nanospheres: a molecular dynamics study. New Journal of Chemistry, 2018, 42, 13619-13628.	1.4	9

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37	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
38	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
39	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
40	Molecular dynamics simulation of anticancer drug delivery from carbon nanotube using metal nanowires. Journal of Computational Chemistry, 2019, 40, 2179-2190.	1.5	8
41	A comparative study of graphite and CNT supported Au-Ag, Au-Pd, Au-Pt and Au-Rh nanoalloys using MD simulation. Journal of Molecular Liquids, 2019, 280, 87-96.	2.3	8
42	Prediction of surface tension of HFD-like fluids using the Fowlerâ€™s approximation. Chemical Physics, 2006, 328, 379-384.	0.9	7
43	Many-body and quantum effects in the surface tension and surface energy of liquid neon and argon using the Fowlerâ€™s approximation. Chemical Physics, 2012, 392, 107-113.	0.9	7
44	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
45	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
46	A comprehensive study of methane/carbon dioxide adsorptive selectivity in different bundle nanotubes. RSC Advances, 2016, 6, 69845-69854.	1.7	7
47	Ptâ€“Co nanocluster in hollow carbon nanospheres. Journal of Computational Chemistry, 2018, 39, 1267-1274.	1.5	7
48	Surface energy, relative stability, and structural properties of Au-Pt, Au-Rh, Au-Cu, and Au-Pd nanoclusters created in inert-gas condensation process using MD simulation. Journal of Physics and Chemistry of Solids, 2020, 144, 109480.	1.9	7
49	Computation of some thermodynamic, structural, and transport properties of fluid oxygen using two-body and three-body intermolecular potentials from molecular dynamics simulation. Chemical Physics, 2010, 377, 115-122.	0.9	6
50	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
51	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
52	Extended many-body potential of Hauschild and Prausnitz for pure HFD-like fluids. Physica A: Statistical Mechanics and Its Applications, 2014, 413, 459-472.	1.2	5
53	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
54	Formation of methane clathrates in carbon nanotubes: a molecular dynamics study. New Journal of Chemistry, 2018, 42, 7083-7095.	1.4	5

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55	Nucleation, coalescence, thermal evolution, and statistical probability of formation of Au/Ir/Pd nanoalloys in gas-phase condensation process. Journal of Molecular Liquids, 2019, 274, 434-446.	2.3	5
56	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
57	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
58	Molecular dynamics investigation on the deliquescence of NH₄Cl and NH₄NO₃nanoparticles under atmospheric conditions. RSC Advances, 2015, 5, 38345-38353.	1.7	3
59	Propene adsorption on goldâ€“palladium nanoalloys supported on bundle nanotubes. RSC Advances, 2016, 6, 66275-66287.	1.7	3
60	Investigation of temperature and pressure effects on thermodynamics and structural properties of gold nanoparticles formed during the gas condensation procedure. Journal of Molecular Liquids, 2019, 281, 39-47.	2.3	3
61	Effective potential for many-body interactions in some properties of the HFD-like solids. Physica A: Statistical Mechanics and Its Applications, 2015, 439, 20-33.	1.2	2
62	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
63	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
64	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
65	Boron Nitride- and Graphene-Supported Trimetallic Yolkâ€“Shell and Hollow Nanoparticles. Industrial & Engineering Chemistry Research, 0, , .	1.8	2
66	Accurate equations of state for CF 4 , CF 4 â€“Ar, and CF 4 â€“CH 4 fluids using two-body and three-body intermolecular potentials from molecular dynamics simulation. Journal of Fluorine Chemistry, 2014, 168, 81-92.	0.9	1
67	A modified thermodynamic insight to deliquescence of a voidâ€containing nanocrystal confirmed by MD simulation. AICHE Journal, 2016, 62, 4066-4077.	1.8	1