Mohsen Abbaspour

List of Publications by Year in Descending Order

66 papers	576 citations	13 h-index	18 g-index
67 ext. papers	684 ext. citations	4.2 avg, IF	4.37 L-index

#	Paper	IF	Citations
66	Ag, Au, Pt, and Au-Pt nanoclusters in [N1114][C1SO3] ionic liquid: A molecular dynamics study. *Journal of Molecular Liquids*, **2022**, 360, 119447	6	1
65	Investigation of doped carbon nanotubes on desalination process using molecular dynamics simulations. *Journal of Molecular Liquids*, **2021**, 348, 118040	6	2
64	Melting Behavior of Bimetallic and Trimetallic Nanoparticles: A Review of MD Simulation Studies. *Topics in Current Chemistry*, **2021**, 379, 22	7.2	2
63	Molecular dynamics simulation of carbon peapod-like nanomaterials in desalination process. *Desalination*, **2021**, 504, 114975	10.3	1
62	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
61	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
60	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
59	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
58	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	3.9	4
57	Molecular dynamics simulation of anticancer drug delivery from carbon nanotube using metal nanowires. *Journal of Computational Chemistry*, **2019**, 40, 2179-2190	3.5	2
56	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	6	5
55	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	6	2
54	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	6	5
53	Au□r nanoalloy nucleation during the gas-phase condensation: a comprehensive MD study including different effects. *Inorganic Chemistry Frontiers*, **2018**, 5, 1445-1457	6.8	12
52	Stability Control of [email□protected] Trimetallic Nanoparticles via Ag□d Core Structure and Composition: A Molecular Dynamics Study. *Industrial & Engineering Chemistry Research*, **2018**, 57, 6236-6245	3.9	3
51	Pt-Co nanocluster in hollow carbon nanospheres. *Journal of Computational Chemistry*, **2018**, 39, 1267-1274	3.5	4
50	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

49	AuFe nanoparticles visited by MD simulation: structural and thermodynamic properties affected by chemical composition. *New Journal of Chemistry*, **2018**, 42, 9666-9675	3.6	8
48	Formation of methane clathrates in carbon nanotubes: a molecular dynamics study. *New Journal of Chemistry*, **2018**, 42, 7083-7095	3.6	2
47	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
46	AgAu nanoparticles encapsulated inside porous hollow carbon nanospheres: a molecular dynamics study. *New Journal of Chemistry*, **2018**, 42, 13619-13628	3.6	5
45	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
44	Density-dependent phase transition in nano-confinement water using molecular dynamics simulation. *Journal of Molecular Liquids*, **2018**, 250, 26-34	6	7
43	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
42	Investigation of Possible Formation of Au@M (M = Cu, Ir, Pt, and Rh) CoreShell Nanoclusters in a CondensationCoalescence Process Using Molecular Dynamics Simulations. *Industrial & Engineering Chemistry Research*, **2018**, 57, 14837-14845	3.9	12
41	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
40	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
39	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
38	Dynamical investigation of formation of Ni Pt nanoclusters in gas phase. *Journal of Molecular Liquids*, **2017**, 240, 221-224	6	18
37	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
36	New molecular insights into the stability of NiPd hollow nanoparticles. *Inorganic Chemistry Frontiers*, **2017**, 4, 1679-1690	6.8	13
35	Structural evolution of Pt/Pd nanoparticles in condensation process. *Journal of Molecular Liquids*, **2017**, 248, 822-829	6	11
34	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
33	A comprehensive study of methane/carbon dioxide adsorptive selectivity in different bundle nanotubes. *RSC Advances*, **2016**, 6, 69845-69854	3.7	4
32	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

31	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
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	5.7	9
29	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
28	Carbon monoxide adsorption on the single-walled carbon nanotube supported goldsilver nanoalloys. *New Journal of Chemistry*, **2016**, 40, 310-319	3.6	9
27	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
26	A modified thermodynamic insight to deliquescence of a void-containing nanocrystal confirmed by MD simulation. *AICHE Journal*, **2016**, 62, 4066-4077	3.6	1
25	Propene adsorption on goldpalladium nanoalloys supported on bundle nanotubes. *RSC Advances*, **2016**, 6, 66275-66287	3.7	3
24	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
23	Molecular dynamics investigation on the deliquescence of NH4Cl and NH4NO3 nanoparticles under atmospheric conditions. *RSC Advances*, **2015**, 5, 38345-38353	3.7	3
22	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
21	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
20	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	3.3	2
19	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
18	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
17	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
16	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
15	Extended many-body potential of Hauschild and Prausnitz for pure HFD-like fluids. *Physica A: Statistical Mechanics and Its Applications*, **2014**, 413, 459-472	3.3	5
14	Accurate equations of state for CF 4 , CF 4 Ar, and CF 4 CH 4 fluids using two-body and three-body intermolecular potentials from molecular dynamics simulation. *Journal of Fluorine Chemistry*, **2014**, 168, 81-92	2.1	1

13	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
12	Many-body and quantum effects in the surface tension and surface energy of liquid neon and argon using the Fowler approximation. *Chemical Physics*, **2012**, 392, 107-113	2.3	7
11	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	2.3	13
10	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	1.9	20
9	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	2.3	6
8	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	1.9	19
7	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	2.3	12
6	Molecular Dynamics Simulation of Argon, Krypton, and Xenon Using Two-Body and Three-Body Intermolecular Potentials. *Journal of Chemical Theory and Computation*, **2006**, 2, 920-6	6.4	28
5	Prediction of surface tension of HFD-like fluids using the Fowler approximation. *Chemical Physics*, **2006**, 328, 379-384	2.3	7
4	Determination of potential energy functions of CO CO, CO2 CO2, and N2O N2O and calculation of their transport properties. *Chemical Physics*, **2006**, 330, 313-325	2.3	12
3	An accurate expression for radial distribution function of the Lennard-Jones fluid. *Chemical Physics*, **2005**, 310, 11-15	2.3	36
2	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	2.5	11
1	Determination of the Potential Energy Function of CF4 CF4 via the Inversion of Reduced Viscosity Collision Integrals at Zero Pressure. *Industrial & Engineering Chemistry Research*, **2003**, 42, 2256-2261	3.9	9