

Curriculum Vitae



Personal Data

Name: Mohsen

Family name: Abbaspour

Nationality: Iranian

Address: Dep. of Chemistry, Hakim Sabzevari University, Sabzevar, Iran

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Education

- Ph. D., Physical Chemistry, June 2006, Ferdowsi University, Mashhad, Iran
- M. S., Physical Chemistry, September 2000, Ferdowsi University, Mashhad, Iran
- B. S., Chemistry, July 1998, Ferdowsi University, Mashhad, Iran

Affiliation

Associated professor of Hakim Sabzevari University

Research Interests

- MD Simulations of nano systems
- Intermolecular potentials
- Transport properties
- MD Simulations of solids, liquids, and gases
- Surface chemistry

Courses Tought

1. General Chemistry 1 & 2
2. Physical Chemistry 1 & 2
3. Surface Chemistry
4. Advanced chemical kinetics
5. Advanced Physical Chemistry
6. Statistical Thermodynamics

Awards

1. Selection of 6th Ferdowsi Festival, Ferdowsi University of Mashhad, 2007.
2. Selection of premier researchers of Hakim Sabzevari University, 2009.
3. Selection of premier researchers of Hakim Sabzevari University, 2017.

Publications

Papers

Thermal stability and melting mechanism of diamond nanothreads: Insight from molecular dynamics simulation

M Eidani, H Akbarzadeh, E Mehrjouei, M Abbaspour, S Salemi, ...

Colloids and Surfaces A: Physicochemical and Engineering Aspects 655, 130248

Formation of methane clathrates into fullerene: A molecular dynamics study

M Abbaspour, H Akbarzadeh, S Salemi, SF Tahami

Journal of Molecular Liquids 367, 120587

2022

Yolk-shell nanoparticles with different cores: A molecular dynamics study

S Ramezanzadeh, H Akbarzadeh, E Mehrjouei, AN Shamkhali, ...

Colloids and Surfaces A: Physicochemical and Engineering Aspects 653, 130019

2022

Molecular insight into C60-grafted graphene oxide as a novel reverse osmosis membrane with low energy consumption for seawater desalination

T Ranjbar, H Akbarzadeh, E Mehrjouei, M Abbaspour, S Salemi, ...

Desalination 542, 116062

2022

Thermal behavior of different types of Au–Pt–Pd nanoparticles: Dumbbell-like, three-shell, core-shell, and random-alloy

H Akbarzadeh, E Mehrjouei, M Abbaspour, S Salemi, H Yaghoubi, ...

Materials Chemistry and Physics, 126955

2022

Ball-Cup, Janus, core-shell and disordered-alloy rhodium-gold nanoparticles: An atomistic simulation on structural stability

H Akbarzadeh, E Mehrjouei, M Abbaspour, S Salemi, H Yaghoubi, ...

Colloids and Surfaces A: Physicochemical and Engineering Aspects 651, 129658

2022

- Ag, Au, Pt, and Au-Pt nanoclusters in [N1114][C1SO3] ionic liquid: A molecular dynamics study 2 2022
 MN Jorabchi, M Abbaspour, EK Goharshadi, S Wohlrab
 Journal of Molecular Liquids 360, 119447
- Ag, Au, Pt, and Au-Pt nanoclusters in [N1114][C1SO3] ionic liquid: A molecular dynamics study 2022
 M Abbaspour, E Kafshdare Goharshadi, S Wohlrab
 Journal of Molecular Liquids 360
- Concave Pd-M (M= Co, Ni, Cu, Rh, Ag, Ir, Pt, and Au) nanocubes explored by molecular dynamics 2 2022
 simulations: A liquid-like expansion mechanism
 H Akbarzadeh, E Mehrjouei, AN Shamkhali, M Abbaspour, C Izanloo, ...
 Applied Surface Science 592, 153203
- Melting Behavior of Bimetallic and Trimetallic Nanoparticles: A Review of MD Simulation Studies
 H Akbarzadeh, E Mehrjouei, M Abbaspour, AN Shamkhali
 Topics in Current Chemistry 379 (3), 1-40
 - Molecular dynamics simulation of carbon peapod-like nanomaterials in desalination process
 M Abbaspour, MN Jorabchi, H Akbarzadeh, N Ahmadi
 Desalination 504, 114975
 - Hierarchical structure in poly (N-vinyl carbazole)/Fe₃O₄ nanocomposites and the relevant magnetic coercivity
 M Abbaspour, H Akbarzadeh, S Salemi, L Bahmanipour
 SOFT MATTER 17 (11), 3085-3095
 - Complex fluids in animal survival strategies
 M Abbaspour, H Akbarzadeh, S Salemi, L Bahmanipour
 SOFT MATTER 17 (11), 3085-3095
 - Stability of Pd@ void@ M (M= Ni, Ag, and Pt) yolk shell nanoparticles controlled by structural factors: A
 molecular dynamics perspective
 H Akbarzadeh, E Mehrjouei, AN Shamkhali, S Ramezanzadeh, ...
 Colloids and Surfaces A: Physicochemical and Engineering Aspects 610, 125920
 - Phase transitions in nanostructured water confined in carbon nanotubes by external electric and magnetic
 fields: a molecular dynamics investigation
 M Abbaspour, H Akbarzadeh, S Salemi, L Bahmanipour
 RSC Advances 11 (18), 10532-10539
 - Structure, dynamics, and morphology of nanostructured water confined between parallel graphene surfaces
 and in carbon nanotubes by applying magnetic and electric fields
 M Abbaspour, H Akbarzadeh, S Salemi, L Bahmanipour
 Soft Matter 17 (11), 3085-3095
 - 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
 Z Valizadeh, M Abbaspour
 Journal of Physics and Chemistry of Solids 144, 109480
 - Investigation of surface energy, stability, and structural behaviors of Au-Ag nanoclusters formed in gas
 condensation process using MD simulation
 M Abbaspour, Z Valizadeh, H Akbarzadeh
 Nashrieh Shimi va Mohandesi Shimi Iran
 - Thermodynamics, Structure, and Dynamic Properties of Nanostructured Water Confined into B-, N-, and Si-
 Doped Graphene Surfaces and Carbon Nanotubes

M Abbaspour, H Akbarzadeh, S Zaeifi
Industrial & Engineering Chemistry Research 59 (20), 9642-9654

- ❑ Molecular dynamics simulation of anticancer drug delivery from carbon nanotube using metal nanowires
M Abbaspour, M Namayandeh Jorabchi, H Akbarzadeh, S Salemi, ...
Journal of computational chemistry 40 (25), 2179-2190
- ❑ Investigation of temperature and pressure effects on thermodynamics and structural properties of gold nanoparticles formed during the gas condensation procedure
S Lotfi, M Abbaspour
Journal of Molecular Liquids 281, 39-47
- ❑ A comparative study of graphite and CNT supported Au-Ag, Au-Pd, Au-Pt and Au-Rh nanoalloys using MD simulation
P Yousefi, M Abbaspour, V Sokhanvaran
Journal of Molecular Liquids 280, 87-96
- ❑ Nucleation, coalescence, thermal evolution, and statistical probability of formation of Au/Ir/Pd nanoalloys in gas-phase condensation process
M Abbaspour, Z Valizadeh, MN Jorabchi
Journal of Molecular Liquids 274, 434-446
- ❑ 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
M Abbaspour, H Akbarzadeh, S Salemi, S Lotfi
Industrial & Engineering Chemistry Research 57 (43), 14837-14845
- ❑ Icosahedral Ir, Rh, Pt, and Cu nanoclusters into gold vapor environment: Thermodynamic and structural analysis of the formed core@ shell nanoclusters using MD simulations
M Abbaspour, H Akbarzadeh, S Lotfi
Journal of Alloys and Compounds 764, 323-332
- ❑ Investigation of different effects on the capacity of supercapacitor comprising an ionic liquid between graphene oxide nanosheets
M Nasimi, H Akbarzadeh, M Abbaspour, S Salemi, V Sokhanvaran, ...
Journal of Molecular Liquids 266, 658-672
- ❑ Unexpected trend for thermodynamic stability of Au@ void@ AgAu yolk-shell nanoparticles: A molecular dynamics study
H Akbarzadeh, E Mehrjouei, AN Shamkhali, M Abbaspour, S Salemi, ...
Applied Surface Science 447, 648-655
- ❑ Pt-Co nanocluster in hollow carbon nanospheres
H Akbarzadeh, M Abbaspour, E Mehrjouei, S Ramezanzadeh
Journal of computational chemistry 39 (19), 1267-1274
- ❑ Stability Control of AgPd@ Pt Trimetallic Nanoparticles via Ag-Pd Core Structure and Composition: A Molecular Dynamics Study
H Akbarzadeh, M Abbaspour, E Mehrjouei, M Kamrani
Industrial & Engineering Chemistry Research 57 (18), 6236-6245
- ❑ Investigation on electrochemical properties of polythiophene nanocomposite with graphite derivatives as supercapacitor material on breath figure-decorated PMMA electrode
M Azimi, M Abbaspour, A Fazli, H Setoodeh, B Pourabbas
Journal of Electronic Materials 47 (3), 2093-2102
- ❑ Molecular dynamics simulation of liquid water and ice nanoclusters using a new effective HFD-like model
M Abbaspour, H Akbarzadeh, S Salemi, K Pirfalak
Journal of computational chemistry 39 (5), 269-278

- ❑ Some properties of solid helium and helium nanoclusters using the effective HFD-like interaction potential: Adsorption and desorption inside carbon nanotube
 M Abbaspour, H Akbarzadeh, SZ Banihashemi, A Sotoudeh
Physica A: Statistical Mechanics and its Applications 491, 219-232
- ❑ Thermodynamic, structural, and dynamical properties of nano-confined water using SPC/E and TIP4P models by molecular dynamics simulations
 E Jalalitalab, M Abbaspour, H Akbarzadeh
New Journal of Chemistry 42 (19), 16258-16272
- ❑ Ag–Au nanoparticles encapsulated inside porous hollow carbon nanospheres: a molecular dynamics study
 H Akbarzadeh, M Abbaspour, E Mehrjouei, S Ramezanzadeh
New Journal of Chemistry 42 (16), 13619-13628
- ❑ Au–Fe nanoparticles visited by MD simulation: structural and thermodynamic properties affected by chemical composition
 H Akbarzadeh, E Mehrjouei, AN Shamkhali, M Abbaspour, S Salemi, ...
New Journal of Chemistry 42 (12), 9666-9675
- ❑ Au–Ir nanoalloy nucleation during the gas-phase condensation: a comprehensive MD study including different effects
 M Abbaspour, H Akbarzadeh, Z Valizadeh
Inorganic Chemistry Frontiers 5 (6), 1445-1457
- ❑ Formation of methane clathrates in carbon nanotubes: a molecular dynamics study
 H Akbarzadeh, M Abbaspour, S Salemi, A Nazarian
New Journal of Chemistry 42 (9), 7083-7095
- ❑ AgPd@ Pt nanoparticles with different morphologies of cuboctahedron, icosahedron, decahedron, octahedron, and Marks-decahedron: insights from atomistic simulations
 H Akbarzadeh, M Abbaspour, E Mehrjouei, M Kamrani
Inorganic Chemistry Frontiers 5 (4), 870-878
- ❑ Density-dependent phase transition in nano-confinement water using molecular dynamics simulation
 M Abbaspour, H Akbarzadeh, S Salemi, E Jalalitalab
Journal of Molecular Liquids 250, 26-34
- ❑ Effect of systematic addition of the third component on the melting characteristics and structural evolution of binary alloy nanoclusters
 H Akbarzadeh, M Abbaspour, E Mehrjouei
Journal of Molecular Liquids 249, 412-419
- ❑ Ag-Nanowire Diffusion into the Carbon Nanotube: an Efficient Method for Anti-Cancer Drug Release
 H Akbarzadeh, E Mehrjouei, M Abbaspour, S Salemi
Nashrieh Shimi va Mohandesi Shimi Iran 36 (4), 189-199
- ❑ Coalescence process of gold/silver core-shell nanoparticles located on carbon nanotube and graphene surfaces
 H Akbarzadeh, M Abbaspour, S Salemi, M Hasani
Journal of Molecular Liquids 248, 738-750
- ❑ Structural evolution of Pt/Pd nanoparticles in condensation process
 H Akbarzadeh, M Abbaspour, E Mehrjouei, A Masoumi
Journal of Molecular Liquids 248, 822-829
- ❑ Injection of mixture of shale gases in a nanoscale pore of graphite and their displacement by CO₂/N₂ gases using molecular dynamics study
 H Akbarzadeh, M Abbaspour, S Salemi, M Akbari
Journal of Molecular Liquids 248, 439-446

- ☐ Au@ void@ AgAu Yolk–Shell Nanoparticles with Dominant Strain Effects: A Molecular Dynamics Simulation
 H Akbarzadeh, E Mehrjouei, AN Shamkhali, M Abbaspour, S Salemi, ...
 The journal of physical chemistry letters 8 (20), 5064-5068
- ☐ 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 ...
 M Abbaspour, H Akbarzadeh, P Yousefi, M Razmkhah
 Journal of colloid and interface science 504, 171-177
- ☐ Solid-state supercapacitor based on breath figured polymethyl methacrylate deposited by graphene: The effect of electrode surface
 M Abbaspour, B Pourabbas, M Azimi, G Abdeali, A Asgari
 Journal of Materials Science: Materials in Electronics 28 (19), 14121-14130
- ☐ Effect of support on the coalescence between Ag@ Au nanoalloys using MD simulations
 H Akbarzadeh, M Abbaspour, S Salemi, M Hasani
 Journal of Molecular Liquids 244, 390-397
- ☐ Au@ Pt and Pt@ Au nanoalloys in the icosahedral and cuboctahedral structures: Which is more stable?
 H Akbarzadeh, M Abbaspour, E Mehrjouei
 Journal of Molecular Liquids 242, 1002-1017
- ☐ Dynamical investigation of formation of NiPt nanoclusters in gas phase
 H Akbarzadeh, M Abbaspour, A Masoumi, E Mehrjouei
 Journal of Molecular Liquids 240, 221-224
- ☐ Delivery of cisplatin anti-cancer drug from carbon, boron nitride, and silicon carbide nanotubes forced by Ag-nanowire: a comprehensive molecular dynamics study
 E Mehrjouei, H Akbarzadeh, AN Shamkhali, M Abbaspour, S Salemi, ...
 Molecular pharmaceutics 14 (7), 2273-2284
- ☐ A comprehensive molecular dynamics investigation on confinement of PtnCum nanocluster inside carbon nanotubes
 H Akbarzadeh, AN Shamkhali, M Abbaspour, S Salemi, Z Attaran
 Colloids and Surfaces A: Physicochemical and Engineering Aspects 522, 433-444
- ☐ Effect of pressure on some properties of Ag@ Pd and Pd@ Ag nanoclusters
 H Akbarzadeh, M Abbaspour
 Journal of Alloys and Compounds 703, 174-179
- ☐ Different morphologies of aluminum nanoclusters: effect of pressure on solid-liquid phase transition of the nanoclusters using molecular dynamics simulations
 H Akbarzadeh, M Abbaspour
 Journal of Molecular Liquids 230, 20-23
- ☐ Effects of pressure, nanoalloy size, and nanoalloy mole fraction on melting of Ir-Rh nanoalloys using molecular dynamics simulations
 H Akbarzadeh, M Abbaspour
 Journal of Alloys and Compounds 694, 1287-1294
- ☐ Effect of Pt addition to AgAu bimetallic nanoclusters: A molecular dynamics study of AgAuPt ternary system
 H Akbarzadeh, AN Shamkhali, M Abbaspour, S Salemi, Z Hajizadeh
 Journal of Alloys and Compounds 692, 647-657
- ☐ New molecular insights into the stability of Ni–Pd hollow nanoparticles
 H Akbarzadeh, E Mehrjouei, AN Shamkhali, M Abbaspour, S Salemi, ...
 Inorganic Chemistry Frontiers 4 (10), 1679-1690

- ❑ Competition between stability of icosahedral and cuboctahedral morphologies in bimetallic nanoalloys
 H Akbarzadeh, M Abbaspour, E Mehrjouei
 Physical Chemistry Chemical Physics 19 (22), 14659-14670
- ❑ AuPd nanoclusters supported on bundles of nanotubes and graphite surface: A comprehensive molecular dynamics study
 H Akbarzadeh, AN Shamkhali, M Abbaspour, S Salemi, E Khomarian
 Journal of Alloys and Compounds 687, 431-441
- ❑ Equation of state and some structural and dynamical properties of the confined Lennard-Jones fluid into carbon nanotube: A molecular dynamics study
 M Abbaspour, H Akbarzadeh, S Salemi, M Abroodi
 Physica A: Statistical Mechanics and its Applications 462, 1075-1090
- ❑ A modified thermodynamic insight to deliquescence of a void-containing nanocrystal confirmed by MD simulation
 H Akbarzadeh, M Abbaspour, S Salemi, A Masoumi, AN Shamkhali
 AIChE Journal 62 (11), 4066-4077
- ❑ Mo nanocluster under high pressure: A molecular dynamics study
 H Akbarzadeh, M Abbaspour
 Journal of Molecular Liquids 222, 648-655
- ❑ Molecular dynamics simulation of noble gas adsorption on graphite: New effective potentials including many-body interactions
 M Abbaspour, H Akbarzadeh, S Salemi, M Sherafati
 Journal of Molecular Liquids 222, 915-922
- ❑ Nanotube diameter dependency of anisotropic pressure of an ionic liquid confined in a carbon nanotube: A molecular dynamics study for [emim][PF6] case
 H Akbarzadeh, M Abbaspour, E Khomarian
 Journal of Molecular Liquids 220, 370-374
- ❑ Investigation of size dependence of the properties of Cu nanoclusters using molecular dynamics simulations
 H Akbarzadeh, M Abbaspour
 Journal of Molecular Liquids 219, 158-164
- ❑ Investigation of melting and freezing of Ag–Au alloy nanoclusters supported on carbon nanotube using molecular dynamics simulations
 H Akbarzadeh, M Abbaspour
 Journal of Molecular Liquids 216, 671-682
- ❑ Investigation of thermal, structural and dynamical properties of $(Au_x-Cu_y-Ni_z) N_{= 32, 108, 256}$ ternary nanosystems: effect of Au addition to Cu–Ni bimetallic nanoclusters ...
 H Akbarzadeh, M Abbaspour, E Mehrjouei
 RSC advances
- ❑ Phase transition in crown-jewel structured Au–Ir nanoalloys with different shapes: a molecular dynamics study
 H Akbarzadeh, M Abbaspour, E Mehrjouei
 Physical Chemistry Chemical Physics 18 (36), 25676-25686
- ❑ A comprehensive study of methane/carbon dioxide adsorptive selectivity in different bundle nanotubes
 H Akbarzadeh, M Abbaspour
 RSC advances 6 (74), 69845-69854
- ❑ A molecular dynamics study of the effect of the substrate on the thermodynamic properties of bound Pt–Cu bimetallic nanoclusters
 H Akbarzadeh, AN Shamkhali, M Abbaspour, S Salemi, Z Attaran
 Physical Chemistry Chemical Physics 18 (31), 21730-21736

- Investigation of thermal, structural and dynamical properties of $(\text{Au}_x\text{-Cu}_y\text{-Ni}_z)$ $N= 32,108,256$ ternary nanosystems: effect of Au addition to Cu–Ni bimetallic nanoclusters via ...
H Akbarzadeh, M Abbaspour, E Mehrjouei
RSC Advances 6 (72), 67619-67629
- Propene adsorption on gold–palladium nanoalloys supported on bundle nanotubes
H Akbarzadeh, M Abbaspour, E Khomarian
RSC advances 6 (70), 66275-66287
- 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 ...
M Abbaspour, H Akbarzadeh, S Salemi, A Sotoudeh
RSC advances 6 (50), 43924-43936
- Carbon monoxide adsorption on the single-walled carbon nanotube supported gold–silver nanoalloys
H Akbarzadeh, M Abbaspour, S Salemi
New Journal of Chemistry 40 (1), 310-319
- Effects of diameter and chirality on structural and dynamical behavior of [EMIM][PF6] encapsulated in carbon nanotube: A molecular dynamics study
H Akbarzadeh, M Abbaspour
Journal of Molecular Liquids 212, 423-429
- Effective potential for many-body interactions in some properties of the HFD-like solids
M Abbaspour, A Farmanbar, Z Borzouie
Physica A: Statistical Mechanics and its Applications 439, 20-33
- Investigation of Thermodynamic, Dynamic, and Structural Properties of H_2 Adsorption on a Ag–Au Nanoalloy with a Carbon Nanotube Support
H Akbarzadeh, M Abbaspour, S Salemi, M Dastoorani
ChemPhysChem 16 (8), 1676-1682
- Molecular dynamics investigation on the deliquescence of NH_4Cl and NH_4NO_3 nanoparticles under atmospheric conditions
H Akbarzadeh, AN Shamkhali, M Abbaspour, S Salemi
- AN EXPRESSION FOR THE RADIAL DISTRIBUTION FUNCTION OF LENNARD-JONES FLUID CONFINED INTO CARBON NANOTUBE
M ABBASPOUR, M ABROODI
- A new and accurate expression for the radial distribution function of confined Lennard-Jones fluid in carbon nanotubes
M Abbaspour, H Akbarzadeh, M Abroodi
RSC advances 5 (116), 95781-95787
- Molecular dynamics investigation on the deliquescence of NH_4Cl and NH_4NO_3 nanoparticles under atmospheric conditions
H Akbarzadeh, AN Shamkhali, M Abbaspour, S Salemi
RSC Advances 5 (48), 38345-38353
- Investigation of thermal evolution of copper nanoclusters encapsulated in carbon nanotubes: a molecular dynamics study
H Akbarzadeh, M Abbaspour, S Salemi, M Abroodi
Physical Chemistry Chemical Physics 17 (19), 12747-12759
- Size dependence of the equation of state for Ne nanoclusters from an effective two-body potential via molecular dynamics simulations
H Akbarzadeh, M Abbaspour
RSC Advances 5 (15), 11297-11308

- ☐ Investigation of the melting of ionic liquid [emim][PF 6] confined inside carbon nanotubes using molecular dynamics simulations
 H Akbarzadeh, M Abbaspour, S Salemi, S Abdollahzadeh
 RSC Advances 5 (5), 3868-3874
- ☐ Accurate equations of state for CF₄, CF₄-Ar, and CF₄-CH₄ fluids using two-body and three-body intermolecular potentials from molecular dynamics simulation
 M Abbaspour, M Sheykh
 Journal of Fluorine Chemistry 168, 81-92
- ☐ Accurate melting temperatures for Ne nanoclusters and bulk from an effective two-body potential via molecular dynamics simulations
 M Abbaspour, H Akbarzadeh
 Fluid Phase Equilibria 381, 90-94
- ☐ Extended many-body potential of Hauschild and Prausnitz for pure HFD-like fluids
 M Abbaspour, N Naderkhovy
 Physica A: Statistical Mechanics and its Applications 413, 459-472
- ☐ Equation of state, elastic constants, and melting curve of solid neon using an effective two-body potential including quantum corrections
 M Abbaspour, Z Borzouie
 Fluid Phase Equilibria 379, 167-174
- ☐ An extended expression for the radial distribution function of HFD-like fluid for investigation of many-body and quantum effects in some transport properties
 M Abbaspour, MN Jorabchi
 Journal of Molecular Liquids 195, 175-181
- ☐ New inversion and ab initio intermolecular potentials for supercritical fluorine: Calculation of some properties and MD simulation
 S Salemi, M Abbaspour, M Ghabdian
 The Journal of Supercritical Fluids 89, 119-127
- ☐ Investigation of Three-Body Interaction of Gas Adsorption on Graphite via Molecular Dynamics Simulation
 M Abbaspour, M Sherafati
- ☐ SIZE EFFECTS ON THE DELIQUESCENCE RELATIVE HUMIDITY OF NH₄ CL NANOPARTICLES: A MOLECULAR DYNAMICS STUDY
 M ABBASPOUR, A ZIYARATI
- ☐ AN EQUATION OF STATE FOR [EMIM][PF 6] CONFINED BETWEEN GRAPHITE WALLS VIA MOLECULAR DYNAMICS SIMULATION
 M ABBASPOUR, E KHOMARIAN, S ABDOLLAHZADEH
- ☐ Many-body effects in some thermodynamic properties of supercritical CO₂, CO₂-Ar, and CO₂-CH₄ using HFD-like potentials from molecular dynamics simulation
 M Abbaspour, E Nameni
 The Journal of Supercritical Fluids 74, 61-69
- ☐ Some properties of fluid fluorine using new two-body and three-body ab initio potentials from molecular dynamics simulation
 M Abbaspour, M Ghabdian, Z Borzouie
- ☐ Calculation of some properties of solid neon using a many-body and quantum corrected HFD-like potential from molecular dynamics simulation
 M Abbaspour, Z Borzouie

- ☐ Many-body and quantum effects in some thermodynamic properties and infinite shear modulus of HFD-like fluid using the radial distribution function
M Abbaspour, A Keyvanloo
Journal of Molecular Liquids 177, 1-6
- ☐ Some thermodynamic properties of fluids SF₆, SF₆-Ar, and SF₆-Kr using new HFD-like potentials including three-body interactions: The inversion method and molecular dynamics ...
M Abbaspour, SN Borj
Fluid phase equilibria 333, 1-12
- ☐ Some thermodynamics and transport properties and new equation of state for fluid hydrogen using a new intermolecular potential
M Abbaspour, S Shakehnia
Journal of Molecular Liquids 170, 51-60
- ☐ Many-body and quantum effects in the surface tension and surface energy of liquid neon and argon using the Fowler's approximation
M Abbaspour
Chemical Physics 392 (1), 107-113
- ☐ Transport, thermodynamic, and structural properties of fluid ammonia using a new intermolecular potential: The inversion method and molecular dynamics simulation
M Abbaspour
Chemical Physics 389 (1-3), 121-127
- ☐ Computation of some thermodynamics, transport, structural properties, and new equation of state for fluid methane using two-body and three-body intermolecular potentials from ...
M Abbaspour
Journal of Molecular Liquids 161 (1), 30-35
- ☐ Computation of some thermodynamic, structural, and transport properties of fluid oxygen using two-body and three-body intermolecular potentials from molecular dynamics simulation
H Ghahremani, M Abbaspour
Chemical Physics 377 (1-3), 115-122
- ☐ Computation of some thermodynamics, transport, structural properties, and new equation of state for fluid neon using a new intermolecular potential from molecular dynamics ...
M Abbaspour, EK Goharshadi
Theoretical Chemistry Accounts 127 (5), 573-585
- ☐ Computation of some thermodynamic properties of helium-neon and helium-krypton fluid mixtures using molecular dynamics simulation
M Abbaspour, EK Goharshadi, MN Jorabchi
Fluid phase equilibria 291 (2), 117-124
- ☐ Computation of some thermodynamic properties of nitrogen using a new intermolecular potential from molecular dynamics simulation
EK Goharshadi, M Abbaspour, MN Jorabchi, M Nahali
Chemical Physics 358 (3), 185-195
- ☐ Quantum computation of the properties of helium using two-body and three-body intermolecular potentials: a molecular dynamics study
EK Goharshadi, M Abbaspour, H Kashani, M Baherololoom
Theoretical Chemistry Accounts 119 (4), 355-368
- ☐ Determination of potential energy functions of CO-CO, CO₂-CO₂, and N₂O-N₂O and calculation of their transport properties
M Abbaspour, EK Goharshadi
Chemical physics 330 (1-2), 313-325

- ☐ Prediction of surface tension of HFD-like fluids using the Fowler's approximation
 EK Goharshadi, M Abbaspour
 Chemical physics 328 (1-3), 379-384
- ☐ Determination of potential energy functions and calculation transport properties of oxygen and nitric oxide via the inversion of reduced viscosity collision integrals at zero ...
 M Abbaspour, EK Goharshadi, JS Emampour
 Chemical physics 326 (2-3), 620-630
- ☐ Molecular dynamics simulation of argon, krypton, and xenon using two-body and three-body intermolecular potentials
 EK Goharshadi, M Abbaspour
 Journal of chemical theory and computation 2 (4), 920-926
- ☐ Molecular dynamics simulation of argon, krypton, and xenon using two-body and three-body intermolecu
 E Kafshdare Goharshadi, M Abbaspour
 Journal of Chemical Theory and Computation
- ☐ An accurate expression for radial distribution function of the Lennard-Jones fluid
 A Morsali, EK Goharshadi, GA Mansoori, M Abbaspour
 Chemical physics 310 (1-3), 11-15
- ☐ New regularities and an equation of state for liquids
 EK Goharshadi, A Morsali, M Abbaspour
 Fluid phase equilibria 230 (1-2), 170-175
- ☐ Diatomic potential energy function for helium
 EK Goharshadi, M Abbaspour
 NISCAIR-CSIR, India
- ☐ Determination of potential energy function of methane via the inversion of reduced viscosity collision integrals at zero pressure
 EK Goharshadi, M Abbaspour
 Fluid phase equilibria 212 (1-2), 53-65
- ☐ Determination of the Potential Energy Function of CF₄-CF₄ via the Inversion of Reduced Viscosity Collision Integrals at Zero Pressure
 EK Goharshadi, M Abbaspour, A Morsali
 Industrial & engineering chemistry research 42 (10), 2256-2261

Proceedings

1. E. K. Goharshadi and M. Abbaspour "Determination of Potential Energy Function of Neon via the Inversion of Reduced Viscosity Collision Integrals at Zero Pressure", The Fourth Congress of Physical Chemistry, Kish, Iran (2001).
2. E. K. Goharshadi and M. Abbaspour "Determination of Potential Energy Function of Helium via the Inversion of Reduced Viscosity Collision Integrals at Zero Pressure", The Fifth Congress of Physical Chemistry, Boushehr, Iran (2002).
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