Ali Maghari

List of Publications by Year
in descending order

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32 papers	430 citations	759233 12 h-index	752698 20 g-index
32 all docs	32 docs citations	32 times ranked	524 citing authors

#	Article	IF	Citations
1	Hydrogen and deuterium separation on metal organic frameworks based on Cu- and Zn-BTC: an experimental and theoretical study. Adsorption, 2021, 27, 925-935.	3.0	8
2	Reaction mechanisms of C(3PJ) and C+(2PJ) with benzene in the interstellar medium from quantum mechanical molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 4205-4216.	2.8	2
3	Reactive molecular dynamics simulation for isotope-exchange reactions in H/D systems: ReaxFFHD development. Journal of Chemical Physics, 2020, 152, 224111.	3.0	2
4	⁴He/³He separation using oxygen-functionalized nanoporous graphene. Physical Chemistry Chemical Physics, 2019, 21, 12414-12422.	2.8	6
5	Interaction mechanism of insulin with ZnO nanoparticles by replica exchange molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3623-3635.	3.5	12
6	Micro-solvation of a bisphosphonate group: an ab initio and effective fragment potential analysis. Structural Chemistry, 2017, 28, 1201-1210.	2.0	1
7	Theoretical investigation of scattering of an atomic projectile confined in a harmonic surface potential. Journal of the Iranian Chemical Society, 2017, 14, 1497-1505.	2.2	3
8	Atomâ€“surface scattering: a comparative study considering real and complex absorbing potentials. Adsorption, 2017, 23, 663-669.	3.0	4
9	Quantum scattering approach for investigation of two interacting atoms trapped in a one-dimensional Morse potential via Lippmann-Schwinger equation. Journal of Mathematical Physics, 2017, 58, 062105.	1.1	1
10	Interaction of insulin with colloidal ZnS quantum dots functionalized by various surface capping agents. Materials Science and Engineering C, 2017, 77, 836-845.	7.3	11
11	Quantum close coupling calculation of transport and relaxation properties for Hg-H 2 system. Chemical Physics, 2016, 479, 99-108.	1.9	4
12	SAFT-VR modelling of the surface and bulk properties of imidazolium and pyridinium based ionic liquids with ten different anions. Journal of Molecular Liquids, 2016, 224, 872-881.	4.9	9
13	Unfolding of insulin at the surface of ZnO quantum dots. International Journal of Biological Macromolecules, 2016, 86, 169-176.	7.5	17
14	Transport properties of methane, ethane, propane, iso-butane and neo-pentane from ab initio potential energy surfaces. Journal of the Iranian Chemical Society, 2016, 13, 1225-1233.	2.2	5
15	Ab initio potential energy curves and transition dipole moments for the low-lying electronic states of NeH+. Computational and Theoretical Chemistry, 2015, 1070, 82-87.	2.5	5
16	Interfacial structure of water/methanol mixture in contact with graphene surface using molecular dynamics simulation. Journal of Statistical Mechanics: Theory and Experiment, 2015, 2015, P06033.	2.3	4
17	Thermophysical properties of alkyl-imidazolium based ionic liquids through the heterosegmented SAFT-BACK equation of state. Journal of Molecular Liquids, 2014, 191, 59-67.	4.9	35
18	Relaxation of a steep density gradient in a simple fluid: Comparison between atomistic and continuum modeling. Journal of Chemical Physics, 2014, 141, 154107.	3.0	10

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19	CF₄decomposition in a low-pressure ICP: influence of applied power and O₂content. Journal Physics D: Applied Physics, 2014, 47, 355205.	2.8	17
20	Non-equilibrium molecular dynamics simulation of thermal conductivity and thermal diffusion of binary mixtures confined in a nanochannel. Chemical Physics, 2014, 444, 30-38.	1.9	9
21	Ab initio potential energy curves and transition dipole moments for the low-lying states of CH+. Computational and Theoretical Chemistry, 2014, 1047, 22-29.	2.5	25
22	Prediction of thermodynamic properties of pure ionic liquids through extended SAFT-BACK equation of state. Fluid Phase Equilibria, 2013, 356, 109-116.	2.5	28
23	Influence of N2 concentration in a CH4/N2 dielectric barrier discharge used for CH4 conversion into H2. International Journal of Hydrogen Energy, 2013, 38, 16098-16120.	7.1	70
24	Binding of Noble Metal Clusters with Rare Gas Atoms: Theoretical Investigation. Journal of Physical Chemistry A, 2012, 116, 12510-12517.	2.5	36
25	Second-order thermodynamic derivative properties of binary mixtures of n-alkanes through the SAFT-CP equation of state. Fluid Phase Equilibria, 2011, 302, 195-201.	2.5	19
26	On the Calculation of Surface Tensions of n-Alkanes Using the Modified SAFT-BACK-DFT Approach. Journal of Solution Chemistry, 2010, 39, 31-41.	1.2	8
27	Calculation of Transport Coefficients for CH4â€“N2and CH4â€“O2by the Inversion Method. Journal of the Physical Society of Japan, 2004, 73, 1191-1196.	1.6	10
28	Nonequilibrium Molecular Dynamics Study of Thermal Diffusion Behavior of the MMSV Potential Model for Hydrogen. Journal of the Physical Society of Japan, 2001, 70, 3261-3267.	1.6	6
29	On the Sensitivity of Thermal Diffusion to the Intermolecular Pair Potential. Journal of the Physical Society of Japan, 2000, 69, 1389-1393.	1.6	12
30	Direct Determination of the Intermolecular Potential for H2â€“H2from a Viscosity Correlation Equation. Journal of the Physical Society of Japan, 1999, 68, 2276-2280.	1.6	17
31	Direct Determination of the Interaction Potentials for SF6-Ar, SF6-Kr and SF6-Xe from the Extended Law of Corresponding States. Journal of the Physical Society of Japan, 1998, 67, 3086-3089.	1.6	20
32	Prediction of Joule-Thomson Inversion Curves from van der Waals Type Equations of State.. Journal of Chemical Engineering of Japan, 1997, 30, 520-525.	0.6	14