Narayan P Adhikari

List of Publications by Year
in descending order

57	718	840776 11	552781 26
papers	citations	h-index	g-index

58	58	58	708
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hierarchical Modeling of Polystyrene: From Atomistic to Coarse-Grained Simulations. Macromolecules, 2006, 39, 6708-6719.	4.8	314
2	Ethylbenzene Diffusion in Polystyrene:â€‰ United Atom Atomistic/Coarse Grained Simulations and Experiments. Macromolecules, 2007, 40, 7026-7035.	4.8	64
3	Temperature dependence of diffusion coefficient of carbon monoxide in water: A molecular dynamics study. Journal of Molecular Liquids, 2014, 194, 77-84.	4.9	33
4	First-principles study of the interaction of hydrogen molecular on Na-adsorbed graphene. Applied Nanoscience (Switzerland), 2015, 5, 393-402.	3.1	24
5	Molecular dynamics study of diffusion of heavy water in normal water at different temperatures. Journal of Molecular Liquids, 2012, 167, 34-39.	4.9	21
6	Multiscale Modeling of the Surfactant Mediated Synthesis and Supramolecular Assembly of Cobalt Nanodots. Physical Review Letters, 2004, 93, 188301.	7.8	19
7	Structure, electronic and magnetic properties of 2D Graphene-Molybdenum diSulphide (G-MoS2) Heterostructure (HS) with vacancy defects at Mo sites. Computational Condensed Matter, 2020, 24, e00489.	2.1	17
8	Mixing behaviour of Niâ€“Al melt at 1873 K. Physics and Chemistry of Liquids, 2016, 54, 370-383.	1.2	16
9	Effects of slip on the viscosity of polymer melts. Journal of Polymer Science, Part B: Polymer Physics, 2004, 42, 1888-1904.	2.1	15
10	A MOLECULAR DYNAMICS STUDY OF OXYGEN GAS IN WATER AT DIFFERENT TEMPERATURES. International Journal of Modern Physics B, 2013, 27, 1350023.	2.0	14
11	First-principles study of the stability of graphene and adsorption of halogen atoms (F,) Tj ETQq1 1 0.784314 rgBT /Over Modern Physics B, 2014, 28, 1450141.	2.0	13
12	Interfacial Properties of Flexible and Semiflexible Polymers. Macromolecular Theory and Simulations, 2002, 11, 315.	1.4	12
13	Temperature dependence of diffusion coefficient of nitrogen gas in water: A molecular dynamics study. International Journal of Modern Physics B, 2014, 28, 1450084.	2.0	12
14	Transport properties of methane, ethane, propane, and n-butane in water. Journal of Physics Communications, 2018, 2, 065003.	1.2	11
15	Hydrogen storage on palladium adsorbed graphene: A density functional theory study. International Journal of Modern Physics B, 2015, 29, 1550143.	2.0	9
16	Transport properties of zwitterion glycine, diglycine, and triglycine in water. AIP Advances, 2019, 9, .	1.3	9
17	First-principles study of structure, electronic, and magnetic properties of C sites vacancy defects in water adsorbed graphene/MoS2 van der Waals heterostructures. Journal of Molecular Modeling, 2021, 27, 82.	1.8	9
18	Diffusion coefficients of nitric oxide in water: A molecular dynamics study. International Journal of Modern Physics B, 2016, 30, 1650205.	2.0	8

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19	Effect of vacancy defects in 2D vdW graphene/h-BN heterostructure: First-principles study. AIP Advances, 2021, 11, .	1.3	8
20	Interfacial Properties of Asymmetric Polymer Mixtures. Macromolecular Theory and Simulations, 2003, 12, 499-507.	1.4	7
21	Study of structural and transport properties of argon, krypton, and their binary mixtures at different temperatures. Journal of Molecular Modeling, 2017, 23, 94.	1.8	7
22	Tuning Structural, Electronic, and Magnetic Properties of C Sites Vacancy Defects in Graphene/MoS2 van der Waals Heterostructure Materials: A First-Principles Study. Advances in Condensed Matter Physics, 2020, 2020, 1-11.	1.1	7
23	Effect of temperature on transport properties of cysteine in water. AIP Advances, 2020, 10, .	1.3	7
24	Binding of SARS-CoV-2/SARS-CoV spike protein with human ACE2 receptor. Journal of Physics Communications, 2021, 5, 035010.	1.2	6
25	MOLECULAR DYNAMICS STUDY OF DIFFUSION OF DIFFERENT INERT GASES LIKE NEON AND ARGON IN WATER AT DIFFERENT TEMPERATURES. International Journal of Modern Physics B, 2012, 26, 1250016.	2.0	5
26	Structural insights into the repair mechanism of AGT for methyl-induced DNA damage. Biological Chemistry, 2021, 402, 1203-1211.	2.5	5
27	Theoretical and experimental study of hydrogen bonded liquids with water as an example. Journal of Molecular Liquids, 2011, 158, 80-91.	4.9	4
28	First-principles Study of Electronic and Magnetic Properties of Manganese Decorated Graphene. Journal of Nepal Physical Society, 2016, 3, 24.	0.2	4
29	First-principles study of electronic and magnetic properties of nickel doped hexagonal boron nitride (h-BN). European Physical Journal B, 2020, 93, 1.	1.5	4
30	Phase separation in mixtures of flexible and semiflexible polymers. Polymer Journal, 2011, 43, 751-756.	2.7	3
31	A study of magnetism in disordered Ptâ€“Mn, Pdâ€“Mn and Niâ€“Mn alloys: an augmented space recursion approach. Journal of Physics Condensed Matter, 2012, 24, 295501.	1.8	3
32	Study of Electronic and Magnetic Properties of CuPd, CuPt, Cu₃Pd and Cu₃Pt: Tight Binding Linear Muffin-Tin Orbitals Approach. Journal of Institute of Science and Technology, 2015, 19, 137-144.	0.5	3
33	Structural, electronic and magnetic properties of S sites vacancy defects graphene/MoS₂ van der Waals heterostructures: First-principles study. International Journal of Computational Materials Science and Engineering, 2021, 10, 2150009.	0.7	3
34	First-principles study of pressure dependence superconductivity in technetium and tantalum. Solid State Communications, 2021, 340, 114526.	1.9	3
35	Thermodynamic and transport properties of amoxicillin. Journal of Molecular Liquids, 2022, 354, 118865.	4.9	3
36	Decomposition of methane hydrates at high pressure: a density-fuctional theory study. High Pressure Research, 2015, 35, 231-238.	1.2	2

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37	First-Principles Study of Molecular Adsorption of Hydrogen/s on Co-Adatom Graphene. Journal of Institute of Science and Technology, 2020, 25, 15-23.	0.5	2
38	Structural, Electronic and Magnetic Properties of Defected Water Adsorbed Single-Layer MoS2. Journal of Institute of Science and Technology, 2021, 26, 43-50.	0.5	2
39	Adsorption of water on C sites vacancy defected graphene/h-BN: First-principles study. Journal of Molecular Modeling, 2022, 28, 107.	1.8	2
40	Electronic structure and magnetic properties of bulk elements (Fe and Pd) and ordered binary alloys (FePd and Fe3Pd):TB-LMTO-ASA. Journal of College of Medical Sciences-Nepal, 0, 11, 60-69.	0.3	1
41	First-principles study of solid methane at high pressure. Journal of College of Medical Sciences-Nepal, 0, 12, 70-79.	0.3	1
42	First-principles study of a molecular adsorption of fluorine on monolayer MoS2. Journal of College of Medical Sciences-Nepal, 0, 13, 50-59.	0.3	1
43	Molecular dynamics study of diffusion of krypton in water at different temperatures. International Journal of Modern Physics B, 2016, 30, 1650064.	2.0	1
44	Electronic and magnetic properties of defected MoS2 monolayer. Journal of College of Medical Sciences-Nepal, 2021, 18, 68-79.	0.3	1
45	Study of Spin Glass Behavior in Disordered PtxMn1â^'x Alloys: An Augmented Space Recursion Approach. Advanced Science Letters, 2015, 21, 2681-2687.	0.2	1
46	Intermolecular Interaction of Hthyni Protein with Double Methylated DNA at 5m-Cytosine Nucleotide. Journal of Institute of Science and Technology, 2020, 25, 37-44.	0.5	1
47	Elastic property of sickle and normal hemoglobin protein: Molecular dynamics. AIP Advances, 2022, 12, .	1.3	1
48	Chapter 4 Multiscale modeling of the synthesis of quantum nanodots and their arrays. Theoretical and Computational Chemistry, 2007, 18, 85-99.	0.4	0
49	Interfacial Tension and Width of an Asymmetric Polymer Mixture. Macromolecular Symposia, 2012, 315, 15-23.	0.7	0
50	Structure and Symmetrization of Hydrogen Bonding in Ices VIII and X at High Pressure: A Density Functional Theory Approach. Journal of Institute of Science and Technology, 2015, 19, 14-18.	0.5	0
51	Transport properties of cysteine dimer in water. Himalayan Physics, 2019, 8, 11-18.	0.3	0
52	Thermal properties of normal and sickled hemoglobin protein. Journal of College of Medical Sciences-Nepal, 2021, 18, 140-148.	0.3	0
53	Molecular dynamics study of structural properties of Î³-aminobutyric acid (GABA). Journal of College of Medical Sciences-Nepal, 2021, 18, 67-74.	0.3	0
54	Basis Set Effect on Alkaline-Earth Fluoride Structures. Journal of Computational and Theoretical Nanoscience, 2017, 14, 2315-2318.	0.4	0

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55	Hydrogen storage on multiple palladium-decorated graphene. International Journal of Modern Physics B, 0, , .	2.0	0
56	Structural and vibrational properties of amines adsorbed on graphene. Nano Structures Nano Objects, 2022, 29, 100816.	3.5	0
57	Adsorption of Water Molecule in Graphene/MoS2 Heterostructure with Vacancy Defects in Mo Sites. Advances in Condensed Matter Physics, 2022, 2022, 1-18.	1.1	0