Vivek K Yadav

List of Publications by Year
in descending order

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27	465	687363 13	713466 21
papers	citations	h-index	g-index

28	28	28	505
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Recent Advances in the Carrier Mobility of Two-Dimensional Materials: A Theoretical Perspective. ACS Omega, 2020, 5, 14203-14211.	3.5	130
2	First-Principles Simulation Study of Vibrational Spectral Diffusion and Hydrogen Bond Fluctuations in Aqueous Solution of N-Methylacetamide. Journal of Physical Chemistry B, 2015, 119, 9858-9867.	2.6	31
3	Boronâ€“Carbonâ€“Nitride Sheet as a Novel Surface for Biological Applications: Insights from Density Functional Theory. ACS Omega, 2019, 4, 3732-3738.	3.5	29
4	Fe₃O₄-Functionalized Boron Nitride Nanosheets as Novel Adsorbents for Removal of Arsenic(III) from Contaminated Water. ACS Omega, 2020, 5, 10301-10314.	3.5	27
5	A first-principles theoretical study of hydrogen-bond dynamics and vibrational spectral diffusion in aqueous ionic solution: Water in the hydration shell of a fluoride ion. Pure and Applied Chemistry, 2012, 85, 27-40.	1.9	26
6	A computational study of structural, electronic and carrier mobility of boron and phosphorus/nitrogen co-doped graphene. Physica B: Condensed Matter, 2019, 571, 291-295.	2.7	19
7	Phonons and thermal conducting properties of borocarbonitride (BCN) nanosheets. Nanoscale, 2018, 10, 22148-22154.	5.6	18
8	Defect-enriched tunability of electronic and charge-carrier transport characteristics of 2D borocarbonitride (BCN) monolayers from ab initio calculations. Nanoscale, 2019, 11, 19398-19407.	5.6	18
9	A first principles molecular dynamics study of vibrational spectral diffusion and hydrogen bond dynamics in liquid methanol. Chemical Physics, 2012, 408, 36-42.	1.9	16
10	Density Functional Theory Study of Aspirin Adsorption on BCN Sheets and their Hydrogen Evolution Reaction Activity: a Comparative Study with Graphene and Hexagonal Boron Nitride. ChemPhysChem, 2019, 20, 687-694.	2.1	16
11	Dynamics of hydrogen bonds and vibrational spectral diffusion in liquid methanol from first principles simulations with dispersion corrected density functional. Chemical Physics, 2013, 415, 1-7.	1.9	15
12	Efficient CO₂ Capture and Activation on Novel Two-Dimensional Transition Metal Borides. ACS Applied Materials & Interfaces, 2022, 14, 29703-29710.	8.0	15
13	Tunable two-dimensional interfacial coupling in molecular heterostructures. Nature Communications, 2017, 8, 312.	12.8	14
14	Dynamics of supercritical methanol of varying density from first principles simulations: Hydrogen bond fluctuations, vibrational spectral diffusion, and orientational relaxation. Journal of Chemical Physics, 2013, 138, 224501.	3.0	13
15	Probing the dynamics of N-methylacetamide in methanol via ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 12868-12875.	2.8	12
16	A simple molecular design for tunable two-dimensional imine covalent organic frameworks for optoelectronic applications. Physical Chemistry Chemical Physics, 2020, 22, 21360-21368.	2.8	11
17	Formaldehyde-mediated spectroscopic properties of heavy water from first principles simulation. Computational and Theoretical Chemistry, 2017, 1122, 9-15.	2.5	8
18	Electronic Structure of a Semiconducting Imineâ€Covalent Organic Framework. Chemistry - an Asian Journal, 2019, 14, 4645-4650.	3.3	8

#	ARTICLE	IF	CITATIONS
19	Bioactive products from singlet oxygen photooxygenation of cannabinoids. European Journal of Medicinal Chemistry, 2018, 143, 983-996.	5.5	7
20	Electronic properties and superior CO2 capture selectivity of metal nitride (XN) and phosphide (XP) (XÂ=ÂAl, Ga and In) sheets. Applied Surface Science, 2020, 527, 146445.	6.1	7
21	Understanding the Adsorption Energetics of Growth Polymorphs of Ferrocene Derivatives: Microscopic Thermal Desorption Analysis. Journal of Physical Chemistry C, 2019, 123, 18488-18494.	3.1	6
22	Unraveling the stacking effect and stability in nanocrystalline antimony through DFT. Journal of Physics and Chemistry of Solids, 2020, 136, 109156.	4.0	5
23	Frequency dependence of the reorientational motion of OD bonds of deuterated methanol in liquid phase: A first principles molecular dynamics study. Journal of Molecular Liquids, 2013, 182, 43-47.	4.9	3
24	Revealing the Limits of Intermolecular Interactions: Molecular Rings of Ferrocene Derivatives on Graphite Surface. Journal of Physical Chemistry Letters, 2020, 11, 297-302.	4.6	3
25	Hydrogen bond dynamics and vibrational spectral diffusion in aqueous solution of formaldehyde: a first principles molecular dynamics study. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	2
26	Vibrational spectral diffusion in supercritical deuterated ammonia from first principles simulations: Roles of hydrogen bonds, free ND modes and inertial rotation of ammonia molecules. Journal of Molecular Liquids, 2018, 269, 896-904.	4.9	2
27	Dynamics of vibrational frequency fluctuations in deuterated liquid ammonia: roles of fluctuating hydrogen bonds and free ND modes. Molecular Simulation, 2018, 44, 1210-1219.	2.0	1