Vivek K Yadav

List of Publications by Year
in descending order

27	465	687220 13	713332 21
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Efficient CO₂ Capture and Activation on Novel Two-Dimensional Transition Metal Borides. ACS Applied Materials & Interfaces, 2022, 14, 29703-29710.	4.0	15
2	Unraveling the stacking effect and stability in nanocrystalline antimony through DFT. Journal of Physics and Chemistry of Solids, 2020, 136, 109156.	1.9	5
3	Revealing the Limits of Intermolecular Interactions: Molecular Rings of Ferrocene Derivatives on Graphite Surface. Journal of Physical Chemistry Letters, 2020, 11, 297-302.	2.1	3
4	A simple molecular design for tunable two-dimensional imine covalent organic frameworks for optoelectronic applications. Physical Chemistry Chemical Physics, 2020, 22, 21360-21368.	1.3	11
5	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.	3.1	7
6	Recent Advances in the Carrier Mobility of Two-Dimensional Materials: A Theoretical Perspective. ACS Omega, 2020, 5, 14203-14211.	1.6	130
7	Fe₃O₄-Functionalized Boron Nitride Nanosheets as Novel Adsorbents for Removal of Arsenic(III) from Contaminated Water. ACS Omega, 2020, 5, 10301-10314.	1.6	27
8	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.	1.3	19
9	Understanding the Adsorption Energetics of Growth Polymorphs of Ferrocene Derivatives: Microscopic Thermal Desorption Analysis. Journal of Physical Chemistry C, 2019, 123, 18488-18494.	1.5	6
10	Electronic Structure of a Semiconducting Imineâ€Covalent Organic Framework. Chemistry - an Asian Journal, 2019, 14, 4645-4650.	1.7	8
11	Defect-enriched tunability of electronic and charge-carrier transport characteristics of 2D borocarbonitride (BCN) monolayers from ab initio calculations. Nanoscale, 2019, 11, 19398-19407.	2.8	18
12	Boronâ€“Carbonâ€“Nitride Sheet as a Novel Surface for Biological Applications: Insights from Density Functional Theory. ACS Omega, 2019, 4, 3732-3738.	1.6	29
13	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.	1.0	16
14	Bioactive products from singlet oxygen photooxygenation of cannabinoids. European Journal of Medicinal Chemistry, 2018, 143, 983-996.	2.6	7
15	Phonons and thermal conducting properties of borocarbonitride (BCN) nanosheets. Nanoscale, 2018, 10, 22148-22154.	2.8	18
16	Hydrogen bond dynamics and vibrational spectral diffusion in aqueous solution of formaldehyde: a first principles molecular dynamics study. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	2
17	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.	2.3	2
18	Dynamics of vibrational frequency fluctuations in deuterated liquid ammonia: roles of fluctuating hydrogen bonds and free ND modes. Molecular Simulation, 2018, 44, 1210-1219.	0.9	1

#	ARTICLE	IF	CITATIONS
19	Probing the dynamics of N-methylacetamide in methanol via ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 12868-12875.	1.3	12
20	Formaldehyde-mediated spectroscopic properties of heavy water from first principles simulation. Computational and Theoretical Chemistry, 2017, 1122, 9-15.	1.1	8
21	Tunable two-dimensional interfacial coupling in molecular heterostructures. Nature Communications, 2017, 8, 312.	5.8	14
22	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.	1.2	31
23	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.	1.2	13
24	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.	0.9	15
25	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.	2.3	3
26	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.	0.9	26
27	A first principles molecular dynamics study of vibrational spectral diffusion and hydrogen bond dynamics in liquid methanol. Chemical Physics, 2012, 408, 36-42.	0.9	16