Thogluva Janardhanan Dhilip Kumar

List of Publications by Year
in descending order

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67 papers	1,495 citations	331538 21 h-index	360920 35 g-index
67 all docs	67 docs citations	67 times ranked	1164 citing authors

#	ARTICLE	IF	CITATIONS
1	Electronic structure calculations and quantum dynamics of rotational deexcitation of CNNC by He. Physical Chemistry Chemical Physics, 2022, 24, 2785-2793.	1.3	8
2	Si doped T-graphene: a 2D lattice as an anode electrode in Na ion secondary batteries. New Journal of Chemistry, 2022, 46, 9718-9726.	1.4	10
3	Rotational quenching of C2 with 3He and 4He collisions at ultracold temperatures. Chemical Physics Letters, 2022, 798, 139623.	1.2	2
4	Catalytic interplay of metal ions (Cu²⁺, Ni²⁺, and Fe²⁺) in MFe₂O₄ inverse spinel catalysts for enhancing the activity and selectivity during selective transfer hydrogenation of furfural into 2-methylfuran. Catalysis Science and Technology, 2022, 12, 4857-4870.	2.1	14
5	Ab initio characterization of N doped T-graphene and its application as an anode material for Na ion rechargeable batteries. Sustainable Energy and Fuels, 2021, 5, 4060-4068.	2.5	9
6	First-principles study of a 2-dimensional C-silicyne monolayer as a promising anode in Na/K ion secondary batteries. Physical Chemistry Chemical Physics, 2021, 23, 11755-11763.	1.3	21
7	Density Functional Theory Study of Li-Functionalized Nanoporous R-Graphyneâ€“Metalâ€“Organic Frameworks for Reversible Hydrogen Storage. ACS Applied Nano Materials, 2021, 4, 3949-3957.	2.4	16
8	Tuning structure, electronic, and catalytic properties of non-metal atom doped Janus transition metal dichalcogenides for hydrogen evolution. Applied Surface Science, 2021, 552, 149146.	3.1	33
9	Substituted 2D Janus WSSe monolayers as efficient nanosensor toward toxic gases. Journal of Applied Physics, 2021, 130, .	1.1	16
10	Quantum Dynamics of Rotational Transitions in CN (X2Î£+) by H+ Collisions. Frontiers in Chemistry, 2021, 9, 790416.	1.8	0
11	Ultracold rotational quenching of NCCN scattering with 3He and 4He. Chemical Physics Letters, 2020, 738, 136819.	1.2	9
12	Interaction of cyanogen (NCCN) with proton: A new ab initio potential energy surface. Chemical Physics Letters, 2020, 761, 138013.	1.2	8
13	Efficient hydrogenolysis of aryl ethers over Ce-MOF supported Pd NPs under mild conditions: mechanistic insight using density functional theoretical calculations. Catalysis Science and Technology, 2020, 10, 6892-6901.	2.1	27
14	Highly efficient visible-light-driven reduction of Cr(<scp>vi</scp>) from water by porphyrin-based metalâ€“organic frameworks: effect of band gap engineering on the photocatalytic activity. Catalysis Science and Technology, 2020, 10, 7724-7733.	2.1	41
15	Electronic Structure Calculations of Reversible Hydrogen Storage in Nanoporous Ti Cluster Frameworks. ACS Applied Nano Materials, 2020, 3, 5575-5582.	2.4	14
16	Signatures of non-trivial band topology in LaAs/LaBi heterostructure. Journal of Physics Condensed Matter, 2020, 32, 395703.	0.7	1
17	Rotational de-excitations of C3H+ (1Î£+) by collision with He: new ab initio potential energy surface and scattering calculations. Monthly Notices of the Royal Astronomical Society, 2020, 494, 5675-5681.	1.6	6
18	Hydrogen storage capacity of low-lying isomer of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>24</mml:m functionalized with Ti. International Journal of Hydrogen Energy, 2020, 45, 9936-9945.	3.8	50

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19	Hydrogen trapping potential of Ca decorated metal-graphyne framework. Energy, 2020, 199, 117453.	4.5	13
20	Reversible hydrogen adsorption in Li functionalized [1,1]paracyclophane. International Journal of Hydrogen Energy, 2020, 45, 12940-12948.	3.8	20
21	First-Principles Design and Investigation of Siligraphene as a Potential Anode Material for Na-Ion Batteries. Journal of Physical Chemistry C, 2020, 124, 11293-11300.	1.5	25
22	Quantum Scattering Calculations for Rotational Excitations of C3 by Hydrogen Atom: Potential Energy Surfaces and Rate Coefficients. Journal of Physical Chemistry A, 2019, 123, 7296-7302.	1.1	7
23	An ab initio study of reversible dihydrogen adsorption in metal decorated Î³-graphyne. Journal of Applied Physics, 2019, 126, .	1.1	19
24	Hydrogen Trapping Efficiency of Li-Decorated Metalâ€“Carbyne Framework: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 15046-15052.	1.5	12
25	BN-analogue of [2,2]paracyclophane functionalized with Sc and Ti for hydrogen storage. International Journal of Hydrogen Energy, 2019, 44, 6663-6673.	3.8	23
26	Sc and Ti-functionalized 4-tert-butylcalix[4]arene as reversible hydrogen storage material. International Journal of Hydrogen Energy, 2019, 44, 12724-12732.	3.8	17
27	Environmentally Friendly, Co-catalyst-Free Chemical Fixation of CO₂ at Mild Conditions Using Dual-Walled Nitrogen-Rich Three-Dimensional Porous Metalâ€“Organic Frameworks. Inorganic Chemistry, 2019, 58, 3925-3936.	1.9	111
28	First principle study of reversible hydrogen storage in Sc grafted Calix[4]arene and Octamethylcalix[4]arene. International Journal of Hydrogen Energy, 2019, 44, 4889-4896.	3.8	19
29	First-principles study of hydrogen storage in metal functionalized [4,4]paracyclophane. International Journal of Hydrogen Energy, 2018, 43, 5680-5689.	3.8	23
30	Hydrogen Storage in Sc and Li Decorated Metalâ€“Inorganic Framework. ACS Applied Energy Materials, 2018, 1, 1328-1336.	2.5	27
31	Paracyclophane functionalized with Sc and Li for hydrogen storage. Chemical Physics Letters, 2018, 692, 253-257.	1.2	22
32	Effect of edge defects on band structure of zigzag graphene nanoribbons. Journal of Applied Physics, 2018, 123, .	1.1	7
33	Quantum dynamics study of rotational transitions of NCCN induced by He collision. Journal of Chemical Physics, 2018, 149, 174312.	1.2	15
34	Bandgap Tunability in a One-Dimensional System. Condensed Matter, 2018, 3, 34.	0.8	0
35	Rational Design of a 3D Mn^{II}â€Metalâ€“Organic Framework Based on a Nonmetallated Porphyrin Linker for Selective Capture of CO₂ and Oneâ€Pot Synthesis of Styrene Carbonates. Chemistry - A European Journal, 2018, 24, 16662-16669.	1.7	65
36	Ab Initio Potential Energy Surfaces of C₃ Collision with Proton and Quantum Dynamics of Rotational Transition. Journal of Physical Chemistry A, 2018, 122, 5437-5444.	1.1	11

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37	Density Functional Theory and ab Initio Molecular Dynamics Investigation of Hydronium Interactions with Graphene. Energy Procedia, 2017, 110, 518-522.	1.8	4
38	Fundamental Study of Reversible Hydrogen Storage in Titanium- and Lithium-Functionalized Calix[4]arene. Journal of Physical Chemistry C, 2017, 121, 8703-8710.	1.5	24
39	Rational Design of a Bifunctional, Twoâ€Fold Interpenetrated Zn^{II}â€Metalâ€“Organic Framework for Selective Adsorption of CO₂ and Efficient Aqueous Phase Sensing of 2,4,6â€Trinitrophenol. Chemistry - A European Journal, 2017, 23, 16204-16212.	1.7	100
40	Electronic Structure Calculations of Hydrogen Storage in Lithium-Decorated Metalâ€“Graphyne Framework. ACS Applied Materials & Interfaces, 2017, 9, 28659-28666.	4.0	56
41	Hydrogen sorption efficiency of titanium decorated calix[4]pyrroles. Physical Chemistry Chemical Physics, 2017, 19, 32566-32574.	1.3	21
42	Ab initio potential energy surfaces of HCS + : A study of the ground and the low-lying excited electronic states. Chemical Physics, 2016, 479, 36-41.	0.9	7
43	Rotational quenching of CS in ultracold 3He collisions. Chemical Physics Letters, 2016, 659, 304-309.	1.2	6
44	Ultracold rotational deexcitation of CO (1Î£+) collision with proton. Chemical Physics Letters, 2016, 660, 43-47.	1.2	6
45	Controlled Smooth Edge Formation of Graphene Nanoribbons. Quantum Matter, 2016, 5, 345-347.	0.2	0
46	Sequential desorption energy of hydrogen from nickel clusters. , 2015, , .		0
47	Nonadiabatic couplings and charge transfer study in H + CS⁺collision using time-dependent quantum dynamics. Molecular Physics, 2015, 113, 3271-3281.	0.8	6
48	Edge configurational effect on band gaps in graphene nanoribbons. Physical Review B, 2015, 91, .	1.1	15
49	Energy controlled edge formation for graphene nano ribbons. AIP Conference Proceedings, 2014, , .	0.3	2
50	Fundamental studies of H2 interaction with MAl3 clusters [M=Li, Sc, Ti, Zr]. Journal of Alloys and Compounds, 2014, 588, 144-152.	2.8	6
51	Hydrogen Sorption Efficiency of Titanium-Functionalized Mgâ€“BN Framework. Journal of Physical Chemistry C, 2014, 118, 10859-10866.	1.5	31
52	A conceptual DFT study of the hydrogen trapping efficiency in metal functionalized BN system. RSC Advances, 2014, 4, 30758-30767.	1.7	21
53	A first-principles study of hydrogen interaction and saturation on ScAl3. Journal of Alloys and Compounds, 2013, 552, 457-462.	2.8	11
54	Low-energy rotational inelastic collisions of H+ + CO system. Journal of Chemical Physics, 2012, 136, 044317.	1.2	5

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55	Hydration of alkynes using BrÃ¶nsted acidic ionic liquids in the absence of Nobel metal catalyst/H2SO4. Journal of Molecular Catalysis A, 2012, 360, 61-70.	4.8	43
56	Geometric and electronic structures of hydrogenated transition metal (Sc, Ti, Zr) clusters. Physical Review B, 2009, 79, .	1.1	24
57	Hydrogen multicenter bonds and reversible hydrogen storage. Journal of Chemical Physics, 2009, 130, 114301.	1.2	23
58	Effect of Co doping on catalytic activity of small Pt clusters. Journal of Chemical Physics, 2008, 128, 124704.	1.2	19
59	Nature of Hydrogen Interaction and Saturation on Small Titanium Clusters. Journal of Physical Chemistry A, 2008, 112, 2846-2854.	1.1	28
60	Structural, energetic, and electronic properties of hydrogenated titanium clusters. Journal of Chemical Physics, 2008, 128, 194714.	1.2	22
61	Growth Pathway of Pt Clusters on Î±-Al₂O₃(0001) Surface. Journal of Physical Chemistry C, 2007, 111, 13786-13793.	1.5	35
62	Evolution of Small Ti Clusters and the Dissociative Chemisorption of H2on Ti. Journal of Physical Chemistry C, 2007, 111, 7494-7500.	1.5	59
63	Low energy H+CO scattering revisited. Astronomy and Astrophysics, 2007, 475, L15-L18.	2.1	30
64	First principles study of small palladium cluster growth and isomerization. International Journal of Quantum Chemistry, 2007, 107, 1632-1641.	1.0	45
65	Computational study of hydrogen storage in organometallic compounds. Journal of Chemical Physics, 2007, 126, 094703.	1.2	89
66	Elastic and charge transfer processes in H++CO collisions. Journal of Chemical Physics, 2006, 124, 034314.	1.2	19
67	Vibrationally inelastic collisions in H[sup +]+CO system: Comparing quantum calculations with experiments. Journal of Chemical Physics, 2004, 121, 191.	1.2	17