

# G P Das

## List of Publications by Year in descending order

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41  
papers

1,544  
citations

430874

18  
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315739

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g-index

42  
all docs

42  
docs citations

42  
times ranked

2210  
citing authors

#	ARTICLE	IF	CITATIONS
1	Ferromagnetism in Fe-doped ZnO nanocrystals: Experiment and theory. <i>Physical Review B</i> , 2007, 75, .	3.2	385
2	Electronic structure and Schottky-barrier heights of (111)NiSi <sub>2</sub> /Si A- and B-type interfaces. <i>Physical Review Letters</i> , 1989, 63, 1168-1171.	7.8	136
3	Transition-Metal Decoration Enhanced Room-Temperature Hydrogen Storage in a Defect-Modulated Graphene Sheet. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10297-10301.	3.1	135
4	Band gap engineering by functionalization of BN sheet. <i>Physical Review B</i> , 2012, 85, .	3.2	135
5	Ferromagnetism in Mn-doped GaN: From clusters to crystals. <i>Physical Review B</i> , 2003, 68, .	3.2	68
6	Quantum size effects in layered VX <sub>2</sub> (X = S, Se) materials: Manifestation of metal to semimetal or semiconductor transition. <i>Journal of Applied Physics</i> , 2015, 117, .	2.5	67
7	First principles design of Li functionalized hydrogenated h-BN nanosheet for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 14437-14446.	7.1	65
8	Third conformer of graphane: A first-principles density functional theory study. <i>Physical Review B</i> , 2011, 83, .	3.2	57
9	h-BN Monolayer on the Ni(111) Surface: A Potential Catalyst for Oxidation. <i>ACS Applied Materials &amp; Interfaces</i> , 2013, 5, 10404-10408.	8.0	46
10	Strain-induced band-gap deformation of H/F passivated graphene and h-BN sheet. <i>Physical Review B</i> , 2011, 84, .	3.2	45
11	Hydrogen Storage in Ti-Decorated BC <sub>4</sub> N Nanotube. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17487-17491.	3.1	37
12	A new triazine based $\pi$ -conjugated mesoporous 2D covalent organic framework: its in vitro anticancer activities. <i>Chemical Communications</i> , 2018, 54, 11475-11478.	4.1	37
13	Magnetism in ZnO nanowire with Fe/Co codoping: First-principles density functional calculations. <i>Physical Review B</i> , 2010, 81, .	3.2	36
14	Anti-Kubas Type Interaction in Hydrogen Storage on a Li Decorated BHNH Sheet: A First-Principles Based Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 3840-3844.	3.1	35
15	First principles prediction of the third conformer of hydrogenated BN sheet. <i>Physica Status Solidi - Rapid Research Letters</i> , 2010, 4, 368-370.	2.4	32
16	Electron doped C <sub>2</sub> N monolayer as efficient noble metal-free catalysts for CO oxidation. <i>Applied Surface Science</i> , 2017, 418, 92-98.	6.1	24
17	Dilute magnetic III-V semiconductor spintronics materials: A first-principles approach. <i>Computational Materials Science</i> , 2006, 36, 84-90.	3.0	23
18	First principles design of divacancy defected graphene nanoribbon based rectifying and negative differential resistance device. <i>AIP Advances</i> , 2015, 5, .	1.3	23

#	ARTICLE	IF	CITATIONS
19	First principles electronic structure of coincidence site epitaxial Ag/Si(111) interface. Physica Status Solidi (B): Basic Research, 2013, 250, 1313-1319.	1.5	17
20	Exploring adsorption and desorption characteristics of molecular hydrogen on neutral and charged Mg nanoclusters: A first principles study. Chemical Physics, 2016, 469-470, 123-131.	1.9	15
21	An extended fractal growth regime in the diffusion limited aggregation including edge diffusion. AIP Advances, 2016, 6, .	1.3	13
22	Electronic structure of epitaxial interfaces. Pramana - Journal of Physics, 1992, 38, 545-639.	1.8	12
23	Electronic structure and magnetic properties of Cr/Sn multilayers. Journal of Magnetism and Magnetic Materials, 2002, 246, 317-326.	2.3	12
24	Density functional calculations of hole induced long ranged ferromagnetic ordering in Mn doped Cd <sub>28</sub> Se <sub>28</sub> nanocluster. Applied Physics Letters, 2010, 96, .	3.3	11
25	First-principles identification of the origin for higher activity of surface doped carbon nanohorn: Impact on hydrogen storage. International Journal of Hydrogen Energy, 2019, 44, 23196-23209.	7.1	10
26	A first-principles study of the III-V semiconductor nanosheets. Physical Chemistry Chemical Physics, 2015, 17, 1039-1046.	2.8	9
27	Negative differential resistance in electron tunneling in ultrathin films near the two-dimensional limit. Journal of Applied Physics, 2013, 113, 034308.	2.5	8
28	Energetics and fragmentation of single-doped tin and lead clusters. Physical Review B, 2009, 79, .	3.2	7
29	Origin of spin polarization in an edge boron doped zigzag graphene nanoribbon: a potential spin filter. Nanotechnology, 2018, 29, 345203.	2.6	7
30	Tuning the electronic and magnetic properties of graphene/h-BN hetero nanoribbon: A first-principles investigation. AIP Advances, 2018, 8, .	1.3	7
31	Computationally exploring the role of S-dopant and S-linker in activating the catalytic efficiency of graphene quantum dot for ORR. Catalysis Today, 2021, 370, 36-45.	4.4	7
32	Optical and vibrational properties of hydrogenated BN-sheet: First principles study. Applied Surface Science, 2013, 284, 638-643.	6.1	6
33	High Temperature Ferromagnetism in Fe-Doped ZnO: a Density Functional Investigation. Materials Transactions, 2007, 48, 2119-2122.	1.2	5
34	Structural and electronic properties of S <sub>n</sub> -1Pb and Pb <sub>n</sub> -1Sn clusters: a theoretical investigation through first principles calculations. European Physical Journal D, 2009, 55, 613-625.	1.3	4
35	3d Transition metal decorated B-C-N composite nanostructures for efficient hydrogen storage: A first-principles study. Bulletin of Materials Science, 2009, 32, 353-360.	1.7	3
36	Calculated Electronic Structures and Schottky Barrier Heights of (111) NiSi <sub>2</sub> /Si A- and B-Type Interfaces. NATO ASI Series Series B: Physics, 1989, , 215-234.	0.2	3

#	ARTICLE	IF	CITATIONS
37	Electronic and magnetic properties of vanadium dichalcogenides: A brief overview on theory and experiment. Journal of Applied Physics, 2022, 131, 190701.	2.5	1
38	Density Functional Calculations of Carrier Induced Ferromagnetism in Co Doped Cd <sub>28</sub> Se <sub>28</sub> Nanocluster. , 2011, , .		0
39	Designing a new class of III-IV-V semiconductor nanosheets. , 2013, , .		0
40	Manifestation of surface and interface properties of Ag overlayer on Si (111). , 2013, , .		0
41	Manifestation of interface-induced effects of two-dimensional MSi <sub>2</sub> /Si(111) quantum heterostructures: A first principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2022, , 115291.	2.7	0