G P Das

List of Publications by Year in descending order

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Version: 2024-02-01

		430874	315739
41	1,544	18	38
papers	citations	h-index	g-index

42	42	42	2210
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Manifestation of interface-induced effects of two-dimensional MSi2/Si(111) quantum heterostructures: A first principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2022, , 115291.	2.7	0
2	Electronic and magnetic properties of vanadium dichalcogenides: A brief overview on theory and experiment. Journal of Applied Physics, 2022, 131, 190701.	2.5	1
3	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
4	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
5	A new triazine based Ï€-conjugated mesoporous 2D covalent organic framework: itsin vitroanticancer activities. Chemical Communications, 2018, 54, 11475-11478.	4.1	37
6	Origin of spin polarization in an edge boron doped zigzag graphene nanoribbon: a potential spin filter. Nanotechnology, 2018, 29, 345203.	2.6	7
7	Tuning the electronic and magnetic properties of graphene/h-BN hetero nanoribbon: A first-principles investigation. AIP Advances, 2018, 8, .	1.3	7
8	Electron doped C2N monolayer as efficient noble metal-free catalysts for CO oxidation. Applied Surface Science, 2017, 418, 92-98.	6.1	24
9	An extended fractal growth regime in the diffusion limited aggregation including edge diffusion. AIP Advances, 2016, 6, .	1.3	13
10	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
11	First principles design of Li functionalized hydrogenated h-BN nanosheet for hydrogen storage. International Journal of Hydrogen Energy, 2016, 41, 14437-14446.	7.1	65
12	First principles design of divacancy defected graphene nanoribbon based rectifying and negative differential resistance device. AIP Advances, 2015, 5, .	1.3	23
13	A first-principles study of the IIIâ€“IVâ€“V semiconductor nanosheets. Physical Chemistry Chemical Physics, 2015, 17, 1039-1046.	2.8	9
14	Quantum size effects in layered VX2 (Xâ€‰=â€‰S, Se) materials: Manifestation of metal to semimetal or semiconductor transition. Journal of Applied Physics, 2015, 117, .	2.5	67
15	Optical and vibrational properties of hydrogenated BN-sheet: First principles study. Applied Surface Science, 2013, 284, 638-643.	6.1	6
16	h-BN Monolayer on the Ni(111) Surface: A Potential Catalyst for Oxidation. ACS Applied Materials & Interfaces, 2013, 5, 10404-10408.	8.0	46
17	Negative differential resistance in electron tunneling in ultrathin films near the two-dimensional limit. Journal of Applied Physics, 2013, 113, 034308.	2.5	8
18	Designing a new class of III-IV-V semiconductor nanosheets. , 2013, , .		0

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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	Manifestation of surface and interface properties of Ag overlayer on Si (111). , 2013, , .		0
21	Anti-Kubas Type Interaction in Hydrogen Storage on a Li Decorated BHNH Sheet: A First-Principles Based Study. Journal of Physical Chemistry C, 2012, 116, 3840-3844.	3.1	35
22	Band gap engineering by functionalization of BN sheet. Physical Review B, 2012, 85, .	3.2	135
23	Third conformer of graphane: A first-principles density functional theory study. Physical Review B, 2011, 83, .	3.2	57
24	Strain-induced band-gap deformation of H/F passivated graphene and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>h</mml:mi></mml:mrow></mml:math>-BN sheet. Physical Review B, 2011, 84, .	3.2	45
25	Density Functional Calculations of Carrier Induced Ferromagnetism in Co Doped Cd[sub 28]Se[sub 28] Nanocluster. , 2011, , .		0
26	Density functional calculations of hole induced long ranged ferromagnetic ordering in Mn doped Cd28Se28 nanocluster. Applied Physics Letters, 2010, 96, .	3.3	11
27	Magnetism in ZnO nanowire with Fe/Co codoping: First-principles density functional calculations. Physical Review B, 2010, 81, .	3.2	36
28	Transition-Metal Decoration Enhanced Room-Temperature Hydrogen Storage in a Defect-Modulated Graphene Sheet. Journal of Physical Chemistry C, 2010, 114, 10297-10301.	3.1	135
29	First principles prediction of the third conformer of hydrogenated BN sheet. Physica Status Solidi - Rapid Research Letters, 2010, 4, 368-370.	2.4	32
30	Energetics and fragmentation of single-doped tin and lead clusters. Physical Review B, 2009, 79, .	3.2	7
31	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
32	Structural and electronic properties of Snn-1Pb and Pbn-1Sn clusters: a theoretical investigation through first principles calculations. European Physical Journal D, 2009, 55, 613-625.	1.3	4
33	Hydrogen Storage in Ti-Decorated BC₄N Nanotube. Journal of Physical Chemistry C, 2008, 112, 17487-17491.	3.1	37
34	High Temperature Ferromagnetism in Fe-Doped ZnO: a Density Functional Investigation. Materials Transactions, 2007, 48, 2119-2122.	1.2	5
35	Ferromagnetism in Fe-doped ZnO nanocrystals: Experiment and theory. Physical Review B, 2007, 75, .	3.2	385
36	Dilute magnetic IIIâ€“V semiconductor spintronics materials: A first-principles approach. Computational Materials Science, 2006, 36, 84-90.	3.0	23

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37	Ferromagnetism in Mn-doped GaN:â€ƒFrom clusters to crystals. Physical Review B, 2003, 68, .	3.2	68
38	Electronic structure and magnetic properties of Cr/Sn multilayers. Journal of Magnetism and Magnetic Materials, 2002, 246, 317-326.	2.3	12
39	Electronic structure of epitaxial interfaces. Pramana - Journal of Physics, 1992, 38, 545-639.	1.8	12
40	Electronic structure and Schottky-barrier heights of (111)NiSi2/Si A- and B-type interfaces. Physical Review Letters, 1989, 63, 1168-1171.	7.8	136
41	Calculated Electronic Structures and Schottky Barrier Heights of (111) NiSi2/Si A- and B-Type Interfaces. NATO ASI Series Series B: Physics, 1989, , 215-234.	0.2	3