Alvaro Miranda

List of Publications by Year in descending order

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61 papers	674 citations	687363 13 h-index	642732 23 g-index
61 all docs	61 docs citations	61 times ranked	449 citing authors

#	Article	IF	Citations
1	Alkali and transition metal atom-functionalized germanene for hydrogen storage: A DFT investigation. International Journal of Hydrogen Energy, 2021, 46, 20245-20256.	7.1	57
2	Molecular Doping and Subsurface Dopant Reactivation in Si Nanowires. Nano Letters, 2010, 10, 3590-3595.	9.1	39
3	Silicon nanowires as potential gas sensors: A density functional study. Sensors and Actuators B: Chemical, 2017, 242, 1246-1250.	7.8	39
4	Hydrogen storage capacities of alkali and alkaline-earth metal atoms on SiC monolayer: A first-principles study. International Journal of Hydrogen Energy, 2021, 46, 20266-20279.	7.1	39
5	Light metal functionalized two-dimensional siligene for high capacity hydrogen storage: DFT study. International Journal of Hydrogen Energy, 2021, 46, 29348-29360.	7.1	38
6	Ab initio study of hydrogen storage on metal-decorated GeC monolayers. International Journal of Hydrogen Energy, 2021, 46, 29261-29271.	7.1	35
7	NH3 capture and detection by metal-decorated germanene: a DFT study. Journal of Materials Science, 2022, 57, 8516-8529.	3.7	35
8	Enhanced reversible hydrogen storage performance of light metal-decorated boron-doped siligene: A DFT study. International Journal of Hydrogen Energy, 2022, 47, 41310-41319.	7.1	26
9	NH3 molecular doping of silicon nanowires grown along the [112], [110], [001], and [111] orientations. Nanoscale Research Letters, 2012, 7, 308.	5.7	24
10	DFT-based study of the bulk tin mixed-halide CsSnI3-Br perovskite. Computational Materials Science, 2020, 178, 109619.	3.0	19
11	Quasi-one-dimensional silicon nanostructures for gas molecule adsorption: a DFT investigation. Applied Surface Science, 2019, 475, 278-284.	6.1	14
12	Theoretical modelling of porous silicon decorated with metal atoms for hydrogen storage. International Journal of Hydrogen Energy, 2020, 45, 26321-26333.	7.1	14
13	Carbon monoxide sensing properties of B-, Al- and Ga-doped Si nanowires. Nanotechnology, 2018, 29, 204001.	2.6	13
14	Lithiation effects on the structural and electronic properties of Si nanowires as a potential anode material. Energy Storage Materials, 2019, 20, 438-445.	18.0	13
15	Tin carbide monolayers decorated with alkali metal atoms for hydrogen storage. International Journal of Hydrogen Energy, 2022, 47, 41329-41335.	7.1	13
16	Quantum confinement effects on electronic properties of hydrogenated 3Câ€“SiC nanowires. Microelectronics Journal, 2009, 40, 796-798.	2.0	12
17	Effects of Morphology on the Electronic Properties of Hydrogenated Silicon Carbide Nanowires. Journal of Nano Research, 2009, 5, 161-167.	0.8	12
18	Electronic properties of fluorinated silicon carbide nanowires. Computational Materials Science, 2016, 111, 294-300.	3.0	12

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19	First principles band gap engineering of [1â€¯1â€¯0] oriented 3C-SiC nanowires. Computational Materials Science, 2018, 142, 268-276.	3.0	12
20	Lithium effect on the electronic properties of porous silicon for energy storage applications: a DFT study. Dalton Transactions, 2018, 47, 7505-7514.	3.3	12
21	CO and CO2 adsorption performance of transition metal-functionalized germanene. Materials Letters, 2021, 300, 130201.	2.6	12
22	Transition metal-decorated germanene for NO, N2 and O2 sensing: A DFT study. Surfaces and Interfaces, 2022, 30, 101886.	3.0	12
23	Interconnection effects on the electronic and optical properties of Ge nanostructures: A semi-empirical approach. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1230-1235.	2.7	11
24	Hydrogen storage on metal decorated pristine siligene and metal decorated boron-doped siligene. Materials Letters, 2021, 293, 129743.	2.6	11
25	Hydrogenated Ge nanocrystals: band gap evolution with increasing size. Brazilian Journal of Physics, 2006, 36, 375-378.	1.4	10
26	Phonon optical modes and electronic properties in diamond nanowires. Microelectronic Engineering, 2012, 90, 92-95.	2.4	10
27	Lithium effects on the mechanical and electronic properties of germanium nanowires. Nanotechnology, 2018, 29, 154004.	2.6	9
28	Quantum confinement effects on the harmfulâ€gasâ€sensing properties of silicon nanowires. International Journal of Quantum Chemistry, 2018, 118, e25713.	2.0	9
29	Gas adsorption enhancement on transition-metal-decorated tin carbide monolayers. Materials Letters, 2021, 298, 130030.	2.6	9
30	Optical matrix elements in tight-binding approach of hydrogenated Si nanowires. Microelectronics Journal, 2009, 40, 456-458.	2.0	7
31	Optical vibrational modes of Ge nanowires: A computational approach. Microelectronic Engineering, 2016, 159, 215-220.	2.4	7
32	Band-gap engineering of halogenated silicon nanowires through molecular doping. Journal of Molecular Modeling, 2017, 23, 314.	1.8	7
33	Effects of surface and confinement on the optical vibrational modes and dielectric function of 3C porous silicon carbide: An ab-initio study. Physica B: Condensed Matter, 2018, 550, 420-427.	2.7	7
34	Theoretical study of the mechanical and electronic properties of [111]-Si nanowires with interstitial lithium. Journal of Materials Science: Materials in Electronics, 2018, 29, 15795-15800.	2.2	6
35	Tin carbide monolayers as potential gas sensors. Materials Letters, 2021, 294, 129751.	2.6	6
36	Controlling stability and electronic properties of small-diameter SiC nanowires by fluorination. International Journal of Nanotechnology, 2015, 12, 218.	0.2	5

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37	Electronic structure and optical vibrational modes of 3C-SiC nanowires. International Journal of Nanotechnology, 2015, 12, 275.	0.2	5
38	Interstitial sodium and lithium doping effects on the electronic and mechanical properties of silicon nanowires: a DFT study. Journal of Molecular Modeling, 2019, 25, 338.	1.8	5
39	Silicon nanowires as acetone-adsorptive media for diabetes diagnosis. Applied Surface Science, 2021, 547, 149175.	6.1	5
40	Mechanical and Electronic Properties of Tin Carbide Nanowires. Physica Status Solidi (A) Applications and Materials Science, 2020, 217, 1900590.	1.8	4
41	Adsorption of urea on metal-functionalized Si nanowires for a potential uremia diagnosis: A DFT study. Materials Letters, 2021, 298, 130016.	2.6	4
42	Hydrogen storage on bidimensional GeC with transition metal adatoms. Materials Letters, 2021, 300, 130239.	2.6	4
43	Adsorption of diatomic gas molecules on transition-metal-decorated GeC monolayers. Journal of Materials Science, 2022, 57, 8455-8463.	3.7	4
44	Perovskite-Type Thin Slabs: A First-Principles Study of Their Magnetic and Electronic Properties. IEEE Magnetics Letters, 2016, 7, 1-3.	1.1	3
45	Bidimensional perovskite systems for spintronic applications. Journal of Molecular Modeling, 2017, 23, 322.	1.8	3
46	Molecular oxygen dissociation on tin carbide monolayers with gold adatoms. Materials Letters, 2021, 293, 129675.	2.6	3
47	Effects of substitutional doping and vacancy formation on the structural and electronic properties of siligene: A DFT study. Materials Letters, 2022, 307, 130993.	2.6	3
48	Electronic Band Structure of Cubic Silicon Carbide Nanowires. Materials Science Forum, 2008, 600-603, 575-578.	0.3	2
49	Hydrogen surface passivation of Si and Ge nanowires: A semiempirical approach. International Journal of Quantum Chemistry, 2010, 110, 2448-2454.	2.0	2
50	Effects of lithium on the electronic properties of porous Ge as anode material for batteries. Journal of Computational Chemistry, 2020, 41, 2653-2662.	3.3	2
51	Fluorinated porous silicon as sensor material for environmentally toxic gases: a first-principles study. Materials Advances, 2021, 2, 1072-1082.	5.4	2
52	Sodium effects on the electronic and structural properties of porous silicon for energy storage. International Journal of Energy Research, 0, , .	4.5	2
53	DFT study of anisotropy effects on the electronic properties of diamond nanowires with nitrogen-vacancy center. Journal of Molecular Modeling, 2017, 23, 292.	1.8	1
54	Effects of Surface in the IR and Raman Spectrum of Porous Silicon Carbide. IOP Conference Series: Materials Science and Engineering, 2020, 840, 012009.	0.6	1

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55	Tunable thermal conductivity of ternary alloy semiconductors from first-principles. Journal Physics D: Applied Physics, 2021, 54, 335302.	2.8	1
56	Theoretical approach to the phonon modes of GaSb nanowires. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 143, 115372.	2.7	1
57	Tunable electronic properties of silicon nanowires as sodiumâ€battery anodes. International Journal of Energy Research, 2022, 46, 17151-17162.	4.5	1
58	Dielectric function in semi-empirical tight-binding theory applied to crystalline diamond. , 2008, , .		0
59	Nanoelectronic properties of Si and Ge: A semi-empirical approximation. , 2009, , .		0
60	Modelling of electronic and phononic states of Ge nanostructures. Microelectronics Journal, 2009, 40, 439-441.	2.0	0
61	Electronic properties of [111] hydrogen passivated Ge nanowires with surface substitutional lithium. IOP Conference Series: Materials Science and Engineering, 2020, 840, 012004.	0.6	0