Victor GarcÃ-a-SuÃ¡rez

List of Publications by Year
in descending order

77 papers	5,432 citations	136950 32 h-index	79698 73 g-index
78 all docs	78 docs citations	78 times ranked	5148 citing authors

#	Article	IF	Citations
1	Towards molecular spintronics. Nature Materials, 2005, 4, 335-339.	27.5	1,204
2	Spin and molecular electronics in atomically generated orbital landscapes. Physical Review B, 2006, 73, .	3.2	623
3	Long-range electron tunnelling in oligo-porphyrin molecular wires. Nature Nanotechnology, 2011, 6, 517-523.	31.5	312
4	Correlations between Molecular Structure and Single-Junction Conductance: A Case Study with Oligo(phenylene-ethynylene)-Type Wires. Journal of the American Chemical Society, 2012, 134, 5262-5275.	13.7	279
5	GOLLUM: a next-generation simulation tool for electron, thermal and spin transport. New Journal of Physics, 2014, 16, 093029.	2.9	269
6	Giant thermopower and figure of merit in single-molecule devices. Physical Review B, 2009, 79, .	3.2	257
7	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
8	Oligoyne Single Molecule Wires. Journal of the American Chemical Society, 2009, 131, 15647-15654.	13.7	206
9	Vacancy-induced magnetism inSnO2: A density functional study. Physical Review B, 2008, 78, .	3.2	195
10	Simplifying the conductance profiles of molecular junctions: the use of the trimethylsilylethynyl moiety as a moleculeâ€“gold contact. Dalton Transactions, 2013, 42, 338-341.	3.3	83
11	Stability and properties of high-buckled two-dimensional tin and lead. Physical Review B, 2014, 90, .	3.2	80
12	Non-trivial length dependence of the conductance and negative differential resistance in atomic molecular wires. Nanotechnology, 2008, 19, 455203.	2.6	78
13	First-Principles Study of Electron Transport through the Single-Molecule Magnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Mn</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2009, 102, 246801.	7.8	77
14	Mechanically controlled quantum interference in graphene break junctions. Nature Nanotechnology, 2018, 13, 1126-1131.	31.5	73
15	Tuning the Electrical Conductivity of Nanotube-Encapsulated Metallocene Wires. Physical Review Letters, 2006, 96, 106804.	7.8	69
16	Solvent Dependence of the Single Molecule Conductance of Oligoyne-Based Molecular Wires. Journal of Physical Chemistry C, 2016, 120, 15666-15674.	3.1	67
17	Systematic pseudopotentials from reference eigenvalue sets for DFT calculations. Computational Materials Science, 2015, 98, 372-389.	3.0	57
18	Conductance Oscillations in Zigzag Platinum Chains. Physical Review Letters, 2005, 95, 256804.	7.8	56

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19	Surface-induced magnetism in C-doped SnO2. Applied Physics Letters, 2010, 96, .	3.3	56
20	From microelectronics to molecular spintronics: an explorer's travelling guide. Journal of Materials Chemistry, 2009, 19, 1696.	6.7	49
21	Spin-state dependent conductance switching in single molecule-graphene junctions. Nanoscale, 2018, 10, 7905-7911.	5.6	46
22	Effects of antidots on the transport properties of graphene nanoribbons. Physical Review B, 2009, 80, .	3.2	45
23	Optimized basis sets for the collinear and non-collinear phases of iron. Journal of Physics Condensed Matter, 2004, 16, 5453-5459.	1.8	44
24	Graphene Sculpturene Nanopores for DNA Nucleobase Sensing. Journal of Physical Chemistry B, 2014, 118, 6908-6914.	2.6	43
25	Single-channel conductance ofH2molecules attached to platinum or palladium electrodes. Physical Review B, 2005, 72, .	3.2	42
26	Stabilizing intrinsic defects in SnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, .	3.2	40
27	Tailoring surface electronic states via strain to control adsorption: O/Cu/Ru(0001). Surface Science, 2004, 550, 65-72.	1.9	37
28	Conformation dependence of molecular conductance: chemistry versus geometry. Journal of Physics Condensed Matter, 2008, 20, 022203.	1.8	37
29	Adverse effects of asymmetric contacts on single molecule conductances of HS(CH2)nCOOH in nanoelectrical junctions. Nanotechnology, 2009, 20, 125203.	2.6	37
30	Quantum interference in single molecule electronic systems. Physical Review B, 2011, 83, .	3.2	37
31	Impact of Fano and Breit-Wigner resonances in the thermoelectric properties of nanoscale junctions. Physical Review B, 2013, 88, .	3.2	35
32	First principles simulations of the magnetic and structural properties of Iron. European Physical Journal B, 2004, 40, 371-377.	1.5	33
33	Predictions for the formation of atomic chains in mechanically controllable break-junction experiments. Physical Review B, 2007, 75, .	3.2	30
34	Redox control of thermopower and figure of merit in phase-coherent molecular wires. Nanotechnology, 2014, 25, 205402.	2.6	30
35	In-situ formation of one-dimensional coordination polymers in molecular junctions. Nature Communications, 2019, 10, 262.	12.8	30
36	Intrinsic magnetism in nanosheets of SnO2: A first-principles study. Journal of Magnetism and Magnetic Materials, 2013, 328, 104-108.	2.3	27

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37	Relationship between strain and the surface electronic structure of Cu(111) films on Ru(0001): Theory and experiment. Physical Review B, 2005, 71, .	3.2	26
38	Spin-filtering effect in the transport through a single-molecule magnet Mn12 bridged between metallic electrodes. Journal of Applied Physics, 2009, 105, .	2.5	26
39	Impact of edge shape on the functionalities of graphene-based single-molecule electronics devices. Physical Review B, 2012, 85, .	3.2	26
40	Synthesis and Singleâ€Molecule Conductance Study of Redoxâ€Active Ruthenium Complexes with Pyridyl and Dihydrobenzo[b]thiophene Anchoring Groups. Chemistry - A European Journal, 2016, 22, 12732-12740.	3.3	26
41	Current rectification in molecular junctions produced by local potential fields. Physical Review B, 2010, 81, .	3.2	25
42	Anisotropic magnetoresistance in atomic chains of iridium and platinum from first principles. Physical Review B, 2009, 79, .	3.2	22
43	Dynamically Stable Topological Phase of Arsenene. Scientific Reports, 2019, 9, 7966.	3.3	21
44	First-principles scheme for spectral adjustment in nanoscale transport. New Journal of Physics, 2011, 13, 053026.	2.9	20
45	Strongly correlated electron physics in nanotube-encapsulated metallocene chains. Physical Review B, 2006, 74, .	3.2	19
46	Effects of bonding type and interface geometry on coherent transport through the single-molecule magnetMn12. Physical Review B, 2010, 81, .	3.2	19
47	Multifunctional nanostructured Co-doped ZnO: Co spatial distribution and correlated magnetic properties. Physical Chemistry Chemical Physics, 2018, 20, 20257-20269.	2.8	19
48	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
49	Universality in the low-voltage transport response of molecular wires physisorbed onto graphene electrodes. Physical Review B, 2013, 87, .	3.2	18
50	Low variability of single-molecule conductance assisted by bulky metalâ€“molecule contacts. RSC Advances, 2016, 6, 75111-75121.	3.6	18
51	Thermoelectricity in vertical graphene-C60-graphene architectures. Scientific Reports, 2017, 7, 11680.	3.3	15
52	Development of spontaneous magnetism and half-metallicity in monolayer MoS2. Journal of Magnetism and Magnetic Materials, 2017, 443, 343-351.	2.3	15
53	The effect of stretching thiylâ€“ and ethynylâ€“Au molecular junctions. Journal of Physics Condensed Matter, 2008, 20, 025207.	1.8	14
54	Nonequilibrium transport response from equilibrium transport theory. Physical Review B, 2012, 86, .	3.2	14

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55	Systematic pseudopotentials from reference eigenvalue sets for DFT calculations: Pseudopotential files. Data in Brief, 2015, 3, 21-23.	1.0	14
56	Tuning the conductance of molecular junctions: Transparent versus tunneling regimes. Physical Review B, 2009, 80, .	3.2	13
57	Functionalized 8 nm Long Aryleneethynylene Molecular Wire with Alkyne Termini. European Journal of Organic Chemistry, 2007, 2007, 5244-5249.	2.4	12
58	Study of the transport properties of a molecular junction as a function of the distance between the leads. Physica Status Solidi (B): Basic Research, 2007, 244, 2443-2447.	1.5	12
59	Impact of dimerization and stretching on the transport properties of molybdenum atomic wires. Nanotechnology, 2010, 21, 095205.	2.6	12
60	Nonuniversal behavior of the parity effect in monovalent atomic wires. Physical Review B, 2006, 73, .	3.2	10
61	Electronic properties of alkali- and alkaline-earth-intercalated silicon nanowires. Physical Review B, 2007, 75, .	3.2	10
62	Localized double phonon scattering and DOS induced thermoelectric enhancement of degenerate nonstoichiometric Li_{1â^'x}NbO₂ compounds. RSC Advances, 2017, 7, 53255-53264.	3.6	10
63	Spin signatures in the electrical response of graphene nanogaps. Nanoscale, 2018, 10, 18169-18177.	5.6	10
64	Structure and electronic properties of molybdenum monatomic wires encapsulated in carbon nanotubes. Journal of Physics Condensed Matter, 2011, 23, 265302.	1.8	8
65	Tailoring the Fermi level of the leads in molecular-electronic devices. Physical Review B, 2008, 78, .	3.2	7
66	Symmetry-induced quantum interference effects in metalloporphyrin wires. Journal of Physics Condensed Matter, 2013, 25, 325501.	1.8	7
67	Distortion induced magnetic phase transition in cubic BaFeO 3. Journal of Magnetism and Magnetic Materials, 2016, 401, 1097-1105.	2.3	7
68	Giant magnetoresistance of nickel-contacted carbon nanotubes. Journal of Physics Condensed Matter, 2007, 19, 042201.	1.8	6
69	Characteristic jump in the electrical properties of aPdâ^•AlNâ^•Si-based device on exposure to hydrogen. Physical Review B, 2007, 75, .	3.2	5
70	Charge and spin transport properties of Mo<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>X</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow	3.2	5
71	2 Electronics without bridging components. Scientific Reports, 2020, 10, 496.	3.3	3
72	On determining defects identity in carbon nanotubes using charge probes. Applied Surface Science, 2016, 373, 13-18.	6.1	2

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73	Effects of acceptor doping on a metalorganic switch: DFT vs. model analysis. Physical Chemistry Chemical Physics, 2018, 20, 13588-13597.	2.8	2
74	Electronic Properties of Metallocene Wires. , 2006, , .		1
75	Classification and prediction of bulk densities of states and chemical attributes with machine learning techniques. Applied Mathematics and Computation, 2022, 412, 126587.	2.2	1
76	Effect of Impurity Adsorption on the Electronic and Transport Properties of Graphene Nanogaps. Materials, 2022, 15, 500.	2.9	1
77	Geometry dependence of the conductance oscillations of monovalent atomic chains. Physica Status Solidi (B): Basic Research, 2007, 244, 677-684.	1.5	0