

# Victor GarcÃ-a-SuÃ;rez

## List of Publications by Year in descending order

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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	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
2	Effect of Impurity Adsorption on the Electronic and Transport Properties of Graphene Nanogaps. Materials, 2022, 15, 500.	2.9	1
3	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
4	Scysta: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
5	Electronics without bridging components. Scientific Reports, 2020, 10, 496.	3.3	3
6	Dynamically Stable Topological Phase of Arsenene. Scientific Reports, 2019, 9, 7966.	3.3	21
7	In-situ formation of one-dimensional coordination polymers in molecular junctions. Nature Communications, 2019, 10, 262.	12.8	30
8	Spin-state dependent conductance switching in single molecule-graphene junctions. Nanoscale, 2018, 10, 7905-7911.	5.6	46
9	Effects of acceptor doping on a metalorganic switch: DFT vs. model analysis. Physical Chemistry Chemical Physics, 2018, 20, 13588-13597.	2.8	2
10	Mechanically controlled quantum interference in graphene break junctions. Nature Nanotechnology, 2018, 13, 1126-1131.	31.5	73
11	Spin signatures in the electrical response of graphene nanogaps. Nanoscale, 2018, 10, 18169-18177.	5.6	10
12	Multifunctional nanostructured Co-doped ZnO: Co spatial distribution and correlated magnetic properties. Physical Chemistry Chemical Physics, 2018, 20, 20257-20269.	2.8	19
13	Thermoelectricity in vertical graphene-C60-graphene architectures. Scientific Reports, 2017, 7, 11680.	3.3	15
14	Development of spontaneous magnetism and half-metallicity in monolayer MoS2. Journal of Magnetism and Magnetic Materials, 2017, 443, 343-351.	2.3	15
15	Localized double phonon scattering and DOS induced thermoelectric enhancement of degenerate nonstoichiometric Li <sub>x</sub> NbO <sub>2</sub> compounds. RSC Advances, 2017, 7, 53255-53264.	3.6	10
16	On determining defects identity in carbon nanotubes using charge probes. Applied Surface Science, 2016, 373, 13-18.	6.1	2
17	Synthesis and Single-Molecule Conductance Study of Redox-Active Ruthenium Complexes with Pyridyl and Dihydrobenzo[ <i>b</i> ]thiophene Anchoring Groups. Chemistry - A European Journal, 2016, 22, 12732-12740.	3.3	26
18	Low variability of single-molecule conductance assisted by bulky metal-molecule contacts. RSC Advances, 2016, 6, 75111-75121.	3.6	18

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19	Solvent Dependence of the Single Molecule Conductance of Oligoynes-Based Molecular Wires. Journal of Physical Chemistry C, 2016, 120, 15666-15674.	3.1	67
20	Distortion induced magnetic phase transition in cubic BaFeO <sub>3</sub> . Journal of Magnetism and Magnetic Materials, 2016, 401, 1097-1105.	2.3	7
21	Systematic pseudopotentials from reference eigenvalue sets for DFT calculations: Pseudopotential files. Data in Brief, 2015, 3, 21-23.	1.0	14
22	Systematic pseudopotentials from reference eigenvalue sets for DFT calculations. Computational Materials Science, 2015, 98, 372-389.	3.0	57
23	GOLLUM: a next-generation simulation tool for electron, thermal and spin transport. New Journal of Physics, 2014, 16, 093029.	2.9	269
24	Stability and properties of high-buckled two-dimensional tin and lead. Physical Review B, 2014, 90, .	3.2	80
25	Redox control of thermopower and figure of merit in phase-coherent molecular wires. Nanotechnology, 2014, 25, 205402.	2.6	30
26	Graphene Sculpture Nanopores for DNA Nucleobase Sensing. Journal of Physical Chemistry B, 2014, 118, 6908-6914.	2.6	43
27	Simplifying the conductance profiles of molecular junctions: the use of the trimethylsilylethynyl moiety as a molecule-€“gold contact. Dalton Transactions, 2013, 42, 338-341.	3.3	83
28	Symmetry-induced quantum interference effects in metalloporphyrin wires. Journal of Physics Condensed Matter, 2013, 25, 325501.	1.8	7
29	Intrinsic magnetism in nanosheets of SnO <sub>2</sub> : A first-principles study. Journal of Magnetism and Magnetic Materials, 2013, 328, 104-108.	2.3	27
30	Universality in the low-voltage transport response of molecular wires physisorbed onto graphene electrodes. Physical Review B, 2013, 87, .	3.2	18
31	Stabilizing intrinsic defects in SnO <sub>2</sub> . Physical Review B, 2013, 87, .	3.2	40
32	Impact of Fano and Breit-Wigner resonances in the thermoelectric properties of nanoscale junctions. Physical Review B, 2013, 88, .	3.2	35
33	Nonequilibrium transport response from equilibrium transport theory. Physical Review B, 2012, 86, .	3.2	14
34	Impact of edge shape on the functionalities of graphene-based single-molecule electronics devices. Physical Review B, 2012, 85, .	3.2	26
35	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
36	Charge and spin transport properties of Mo <sub>2</sub> X <sub>2</sub> C <sub>2</sub> . Physical Review B, 2012, 85, .	3.2	14

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37	Structure and electronic properties of molybdenum monatomic wires encapsulated in carbon nanotubes. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 265302.	1.8	8
38	Quantum interference in single molecule electronic systems. <i>Physical Review B</i> , 2011, 83, .	3.2	37
39	Long-range electron tunnelling in oligo-porphyrin molecular wires. <i>Nature Nanotechnology</i> , 2011, 6, 517-523.	31.5	312
40	First-principles scheme for spectral adjustment in nanoscale transport. <i>New Journal of Physics</i> , 2011, 13, 053026.	2.9	20
41	Effects of bonding type and interface geometry on coherent transport through the single-molecule magnet Mn <sub>12</sub> . <i>Physical Review B</i> , 2010, 81, .	3.2	19
42	Current rectification in molecular junctions produced by local potential fields. <i>Physical Review B</i> , 2010, 81, .	3.2	25
43	Impact of dimerization and stretching on the transport properties of molybdenum atomic wires. <i>Nanotechnology</i> , 2010, 21, 095205.	2.6	12
44	Surface-induced magnetism in C-doped SnO <sub>2</sub> . <i>Applied Physics Letters</i> , 2010, 96, .	3.3	56
45	Anisotropic magnetoresistance in atomic chains of iridium and platinum from first principles. <i>Physical Review B</i> , 2009, 79, .	3.2	22
46	Tuning the conductance of molecular junctions: Transparent versus tunneling regimes. <i>Physical Review B</i> , 2009, 80, .	3.2	13
47	Adverse effects of asymmetric contacts on single molecule conductances of HS(CH <sub>2</sub> ) <sub>n</sub> COOH in nanoelectrical junctions. <i>Nanotechnology</i> , 2009, 20, 125203.	2.6	37
48	Spin-filtering effect in the transport through a single-molecule magnet Mn <sub>12</sub> bridged between metallic electrodes. <i>Journal of Applied Physics</i> , 2009, 105, .	2.5	26
49	Oligoynes Single Molecule Wires. <i>Journal of the American Chemical Society</i> , 2009, 131, 15647-15654.	13.7	206
50	Effects of antidots on the transport properties of graphene nanoribbons. <i>Physical Review B</i> , 2009, 80, .	3.2	45
51	From microelectronics to molecular spintronics: an explorer's travelling guide. <i>Journal of Materials Chemistry</i> , 2009, 19, 1696.	6.7	49
52	Giant thermopower and figure of merit in single-molecule devices. <i>Physical Review B</i> , 2009, 79, .	3.2	257
53	First-Principles Study of Electron Transport through the Single-Molecule Magnet $\langle \text{Mn} \rangle_{12}$ . <i>Physical Review Letters</i> , 2009, 102, 246801.	7.8	77
54	Conformation dependence of molecular conductance: chemistry versus geometry. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 022203.	1.8	37

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55	The effect of stretching thiylâ€ and ethynylâ€ Au molecular junctions. Journal of Physics Condensed Matter, 2008, 20, 025207.	1.8	14
56	Vacancy-induced magnetism in SnO <sub>2</sub> : A density functional study. Physical Review B, 2008, 78, .	3.2	195
57	Non-trivial length dependence of the conductance and negative differential resistance in atomic molecular wires. Nanotechnology, 2008, 19, 455203.	2.6	78
58	Tailoring the Fermi level of the leads in molecular-electronic devices. Physical Review B, 2008, 78, .	3.2	7
59	Characteristic jump in the electrical properties of a Pd <sup>+</sup> •AlN <sup>+</sup> •Si-based device on exposure to hydrogen. Physical Review B, 2007, 75, .	3.2	5
60	Electronic properties of alkali- and alkaline-earth-intercalated silicon nanowires. Physical Review B, 2007, 75, .	3.2	10
61	Predictions for the formation of atomic chains in mechanically controllable break-junction experiments. Physical Review B, 2007, 75, .	3.2	30
62	Giant magnetoresistance of nickel-contacted carbon nanotubes. Journal of Physics Condensed Matter, 2007, 19, 042201.	1.8	6
63	Functionalized 8 nm Long Aryleneethynylene Molecular Wire with Alkyne Termini. European Journal of Organic Chemistry, 2007, 2007, 5244-5249.	2.4	12
64	Geometry dependence of the conductance oscillations of monovalent atomic chains. Physica Status Solidi (B): Basic Research, 2007, 244, 677-684.	1.5	0
65	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
66	Electronic Properties of Metallocene Wires. , 2006, , .		1
67	Spin and molecular electronics in atomically generated orbital landscapes. Physical Review B, 2006, 73, .	3.2	623
68	Nonuniversal behavior of the parity effect in monovalent atomic wires. Physical Review B, 2006, 73, .	3.2	10
69	Tuning the Electrical Conductivity of Nanotube-Encapsulated Metallocene Wires. Physical Review Letters, 2006, 96, 106804.	7.8	69
70	Strongly correlated electron physics in nanotube-encapsulated metallocene chains. Physical Review B, 2006, 74, .	3.2	19
71	Towards molecular spintronics. Nature Materials, 2005, 4, 335-339.	27.5	1,204
72	Single-channel conductance of H <sub>2</sub> molecules attached to platinum or palladium electrodes. Physical Review B, 2005, 72, .	3.2	42

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73	Conductance Oscillations in Zigzag Platinum Chains. <i>Physical Review Letters</i> , 2005, 95, 256804.	7.8	56
74	Relationship between strain and the surface electronic structure of Cu(111) films on Ru(0001): Theory and experiment. <i>Physical Review B</i> , 2005, 71, .	3.2	26
75	Optimized basis sets for the collinear and non-collinear phases of iron. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 5453-5459.	1.8	44
76	First principles simulations of the magnetic and structural properties of Iron. <i>European Physical Journal B</i> , 2004, 40, 371-377.	1.5	33
77	Tailoring surface electronic states via strain to control adsorption: O/Cu/Ru(0001). <i>Surface Science</i> , 2004, 550, 65-72.	1.9	37