

Rafael Gutierrez

List of Publications by Year in descending order

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119
papers

3,534
citations

147566
31
h-index

155451
55
g-index

120
all docs

120
docs citations

120
times ranked

3578
citing authors

#	ARTICLE	IF	CITATIONS
1	Spin Specific Electron Conduction through DNA Oligomers. Nano Letters, 2011, 11, 4652-4655.	4.5	323
2	Spin-selective transport through helical molecular systems. Physical Review B, 2012, 85, .	1.1	194
3	Tuning the conductance of a molecular switch. Nature Nanotechnology, 2007, 2, 176-179.	15.6	188
4	Chirality-Dependent Electron Spin Filtering by Molecular Monolayers of Helicenes. Journal of Physical Chemistry Letters, 2018, 9, 2025-2030.	2.1	154
5	Dynamic and Electronic Transport Properties of DNA Translocation through Graphene Nanopores. Nano Letters, 2013, 13, 1969-1976.	4.5	115
6	Incoherent Electron-Phonon Scattering in Octanethiols. Nano Letters, 2004, 4, 2109-2114.	4.5	106
7	Modeling Spin Transport in Helical Fields: Derivation of an Effective Low-Dimensional Hamiltonian. Journal of Physical Chemistry C, 2013, 117, 22276-22284.	1.5	103
8	Engineering the figure of merit and thermopower in single-molecule devices connected to semiconducting electrodes. Physical Review B, 2010, 81, .	1.1	91
9	Anisotropic Thermoelectric Response in Two-Dimensional Puckered Structures. Journal of Physical Chemistry C, 2016, 120, 18841-18849.	1.5	84
10	Theory of an all-carbon molecular switch. Physical Review B, 2002, 65, .	1.1	81
11	Charge Transport through Biomolecular Wires in a Solvent: Bridging Molecular Dynamics and Model Hamiltonian Approaches. Physical Review Letters, 2009, 102, 208102.	2.9	80
12	A Chirality-Based Quantum Leap. ACS Nano, 2022, 16, 4989-5035.	7.3	74
13	Enhanced Magnetoresistance in Chiral Molecular Junctions. Journal of Physical Chemistry Letters, 2018, 9, 5453-5459.	2.1	69
14	Quantum Transport through a DNA Wire in a Dissipative Environment. Nano Letters, 2005, 5, 1093-1097.	4.5	68
15	Effect of oxygen on the growth of (101̄,0) GaN surfaces: The formation of nanpipes. Applied Physics Letters, 1998, 73, 3530-3532.	1.5	66
16	Stoichiometric and non-stoichiometric (101̄,0) and (112̄,0) surfaces in 2H-SiC: a theoretical study. Solid State Communications, 1999, 111, 459-464.	0.9	66
17	Inelastic quantum transport in a ladder model: Implications for DNA conduction and comparison to experiments on suspended DNA oligomers. Physical Review B, 2006, 74, .	1.1	65
18	Organic Zener Diodes: Tunneling across the Gap in Organic Semiconductor Materials. Nano Letters, 2010, 10, 4929-4934.	4.5	64

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19	Dissipative effects in the electronic transport through DNA molecular wires. <i>Physical Review B</i> , 2005, 71, .	1.1	59
20	Structural fluctuations and quantum transport through DNA molecular wires: a combined molecular dynamics and model Hamiltonian approach. <i>New Journal of Physics</i> , 2010, 12, 023022.	1.2	53
21	Observation of “Stick” and “Handle” Intermediates along the Fullerene Road. <i>Physical Review Letters</i> , 2000, 84, 2421-2424.	2.9	52
22	Ionization energies and Coulomb explosion of highly charged C60. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1996, 211, 357-362.	0.9	48
23	Contact effects in spin transport along double-helical molecules. <i>Physical Review B</i> , 2014, 89, .	1.1	46
24	Chirality-Induced Spin Selectivity in a Coarse-Grained Tight-Binding Model for Helicene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27230-27241.	1.5	44
25	Vibrational effects in the linear conductance of carbon nanotubes. <i>Europhysics Letters</i> , 2005, 71, 438-444.	0.7	38
26	Guanosine-based hydrogen-bonded 2D scaffolds: metal-free formation of G-quartet and G-ribbon architectures at the solid/liquid interface. <i>Chemical Communications</i> , 2015, 51, 11677-11680.	2.2	38
27	Ball-and-Chain Dimers from a Hot Fullerene Plasma. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5275-5284.	1.1	37
28	Interaction of Oxygen with Threading Dislocations in GaN. <i>Physica Status Solidi A</i> , 1999, 171, 167-173.	1.7	36
29	Role of Exchange Interactions in the Magnetic Response and Intermolecular Recognition of Chiral Molecules. <i>Nano Letters</i> , 2020, 20, 7077-7086.	4.5	35
30	Atomically Precise Prediction of 2D Self-Assembly of Weakly Bonded Nanostructures: STM Insight into Concentration-Dependent Architectures. <i>Small</i> , 2016, 12, 343-350.	5.2	33
31	Electronic transport through occupied and unoccupied states of an organic molecule on Au: Experiment and theory. <i>Physical Review B</i> , 2002, 65, .	1.1	32
32	Thermal bridging of graphene nanosheets via covalent molecular junctions: A non-equilibrium Green’s functions density functional tight-binding study. <i>Nano Research</i> , 2019, 12, 791-799.	5.8	29
33	Thermal Decoherence and Disorder Effects on Chiral-Induced Spin Selectivity. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5753-5758.	2.1	28
34	Giant magnetoresistance of multiwall carbon nanotubes: Modeling the tube/ferromagnetic-electrode burying contact. <i>Physical Review B</i> , 2004, 69, .	1.1	27
35	Enhancement of thermal transport properties of asymmetric Graphene/hBN nanoribbon heterojunctions by substrate engineering. <i>Carbon</i> , 2017, 124, 642-650.	5.4	27
36	Modeling charge transport in DNA using multi-scale methods. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 2277-2287.	0.7	26

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37	Switchable Negative Differential Resistance Induced by Quantum Interference Effects in Porphyrin-based Molecular Junctions. Journal of Physical Chemistry Letters, 2015, 6, 3950-3955.	2.1	26
38	In-Situ Stretching Patterned Graphene Nanoribbons in the Transmission Electron Microscope. Scientific Reports, 2017, 7, 211.	1.6	26
39	A parabolic model to control quantum interference in T-shaped molecular junctions. Physical Chemistry Chemical Physics, 2013, 15, 13951.	1.3	25
40	Effective Hamiltonian model for helically constrained quantum systems within adiabatic perturbation theory: Application to the chirality-induced spin selectivity (CISS) effect. Journal of Chemical Physics, 2020, 152, 214105.	1.2	24
41	Conductance of a molecular junction mediated by unconventional metal-induced gap states. Europhysics Letters, 2003, 62, 90-96.	0.7	23
42	Stability of silicon carbide structures: from clusters to solid surfaces. Journal of Materials Chemistry, 1996, 6, 1657-1663.	6.7	22
43	Electrical transport properties of small sodium clusters. Physical Review A, 2001, 64, .	1.0	22
44	Reconstructions of the Si-terminated (100) surface in α -SiC: A theoretical study. Physical Review B, 1999, 60, 1771-1776.	1.1	20
45	Copper Induced Conformational Changes of Tripeptide Monolayer Based Impedimetric Biosensor. Scientific Reports, 2017, 7, 9498.	1.6	20
46	Polymerization driven monomer passage through monolayer chemical vapour deposition graphene. Nature Communications, 2018, 9, 4051.	5.8	20
47	Molecular design driving tetraporphyrin self-assembly on graphite: a joint STM, electrochemical and computational study. Nanoscale, 2016, 8, 13678-13686.	2.8	19
48	Tuning quantum electron and phonon transport in two-dimensional materials by strain engineering: a Green's function based study. Physical Chemistry Chemical Physics, 2017, 19, 1487-1495.	1.3	19
49	A theoretical study of O chemisorption on GaN (0001)/(0001 $\bar{1}$,) surfaces. Solid State Communications, 1998, 108, 953-958.	0.9	18
50	Fullerene based devices for molecular electronics. Physica E: Low-Dimensional Systems and Nanostructures, 2002, 12, 749-752.	1.3	18
51	Charge migration through DNA molecules in the presence of mismatches. Physical Review B, 2010, 82, .	1.1	18
52	Light-Induced Contraction/Expansion of 1D Photoswitchable Metallopolymer Monitored at the Solid-Liquid Interface. Small, 2017, 13, 1701790.	5.2	18
53	First-Principle-Based Phonon Transport Properties of Nanoscale Graphene Grain Boundaries. Advanced Science, 2018, 5, 1700365.	5.6	17
54	Probing Charge Transport in Oxidatively Damaged DNA Sequences under the Influence of Structural Fluctuations. Journal of Physical Chemistry B, 2012, 116, 10977-10985.	1.2	16

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55	Engineering thermal rectification in MoS ₂ nanoribbons: a non-equilibrium molecular dynamics study. RSC Advances, 2015, 5, 54345-54351.	1.7	16
56	Distance-dependent coherent charge transport in DNA: crossover from tunneling to free propagation. Journal of Biophysical Chemistry, 2010, 01, 77-85.	0.1	16
57	Conductance Properties of Stilbenoid Molecules. ChemPhysChem, 2003, 4, 1252-1256.	1.0	15
58	Reverse breakdown behavior in organic pin-diodes comprising C60 and pentacene: Experiment and theory. Organic Electronics, 2013, 14, 193-199.	1.4	15
59	Green function, quasi-classical Langevin and Kuboâ€“Greenwood methods in quantum thermal transport. Journal of Physics Condensed Matter, 2019, 31, 273003.	0.7	15
60	Charge Migration in Organic Materials: Can Propagating Charges Affect the Key Physical Quantities Controlling Their Motion?. Israel Journal of Chemistry, 2012, 52, 452-460.	1.0	14
61	Towards synthetic neural networks: can artificial electrochemical neurons be coupled with artificial memristive synapses?. Japanese Journal of Applied Physics, 2020, 59, SI0801.	0.8	14
62	Probing Silicaâ€“Biomolecule Interactions by Solid-State NMR and Molecular Dynamics Simulations. Langmuir, 2016, 32, 11698-11705.	1.6	13
63	Electron Transport through Self-Assembled Monolayers of Tripeptides. Journal of Physical Chemistry C, 2019, 123, 9600-9608.	1.5	13
64	Mechanical Transmission of Rotational Motion between Molecular-Scale Gears. Physical Review Applied, 2020, 13, .	1.5	13
65	Thermoelectric properties of functionalized graphene grain boundaries. Journal of Self-Assembly and Molecular Electronics (SAME), 2015, 2015, 1-20.	0.0	13
66	Dynamical bistability of single-molecule junctions: A combined experimental and theoretical study of PTCDA on Ag(111). Physical Review B, 2011, 84, .	1.1	12
67	Prediction of quantum interference in molecular junctions using a parabolic diagram: Understanding the origin of Fano and anti- resonances. Journal of Physics: Conference Series, 2013, 427, 012013.	0.3	12
68	Quantum Phonon Transport in Nanomaterials: Combining Atomistic with Non-Equilibrium Greenâ€™s Function Techniques. Entropy, 2019, 21, 735.	1.1	12
69	ITO Work Function Tunability by Polarizable Chromophore Monolayers. Langmuir, 2019, 35, 2997-3004.	1.6	12
70	Current-induced rotations of molecular gears. Journal of Physics Communications, 2019, 3, 025011.	0.5	12
71	Understanding the UV luminescence of zinc germanate: The role of native defects. Acta Materialia, 2020, 196, 626-634.	3.8	12
72	Quantum interference based Boolean gates in dangling bond loops on Si(100):H surfaces. Scientific Reports, 2015, 5, 14136.	1.6	11

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73	Interplay between Mechanical and Electronic Degrees of Freedom in π -Stacked Molecular Junctions: From Single Molecules to Mesoscopic Nanoparticle Networks. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6344-6355.	1.5	11
74	Doping of graphene induced by boron/silicon substrate. <i>Nanotechnology</i> , 2017, 28, 215701.	1.3	11
75	A zinc selective oxytocin based biosensor. <i>Journal of Materials Chemistry B</i> , 2020, 8, 155-160.	2.9	11
76	Spin-orbit coupling in nearly metallic chiral carbon nanotubes: a density-functional based study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8848-8853.	1.3	10
77	Molecular and Ionic Dipole Effects on the Electronic Properties of Si/SiO ₂ -Grafted Alkylamine Monolayers. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 44873-44879.	4.0	10
78	Diversification of Device Platforms by Molecular Layers: Hybrid Sensing Platforms, Monolayer Doping, and Modeling. <i>Langmuir</i> , 2018, 34, 14103-14123.	1.6	10
79	Doping engineering of thermoelectric transport in BNC heteronanotubes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1904-1911.	1.3	10
80	Spin-Polarized Electron Transmission in DNA-Like Systems. <i>Biomolecules</i> , 2020, 10, 49.	1.8	10
81	Interactions of Long-Chain Polyamines with Silica Studied by Molecular Dynamics Simulations and Solid-State NMR Spectroscopy. <i>Langmuir</i> , 2020, 36, 11600-11609.	1.6	9
82	The contribution of intermolecular spin interactions to the London dispersion forces between chiral molecules. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	9
83	Contact effects and quantum interference in engineered dangling bond loops on silicon surfaces. <i>Nanoscale</i> , 2015, 7, 13967-13973.	2.8	8
84	Discrete polygonal supramolecular architectures of isocytosine-based Pt(κ scp) complexes at the solution/graphite interface. <i>Chemical Communications</i> , 2016, 52, 11163-11166.	2.2	8
85	Direct Assembly and Metal-Ion Binding Properties of Oxytocin Monolayer on Gold Surfaces. <i>Langmuir</i> , 2019, 35, 11114-11122.	1.6	8
86	Coherent spin dynamics in a helical arrangement of molecular dipoles. <i>AIMS Materials Science</i> , 2017, 4, 1052-1061.	0.7	8
87	Conductance Calculations for Real Systems on the Nanoscale. <i>ChemPhysChem</i> , 2002, 3, 650.	1.0	7
88	SCREW MOTION OF DNA DUPLEX DURING TRANSLOCATION THROUGH PORE I: INTRODUCTION OF THE COARSE-GRAINED MODEL. <i>Biophysical Reviews and Letters</i> , 2009, 04, 209-230.	0.9	7
89	Heat transport and thermal rectification in molecular junctions: A minimal model approach. <i>Physical Review B</i> , 2011, 84, .	1.1	7
90	Structural distortions in molecular-based quantum cellular automata: a minimal model based study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17777-17785.	1.3	7

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91	Impact of device geometry on electron and phonon transport in graphene nanorings. Physical Review B, 2019, 99, .	1.1	7
92	Selective Transmission of Phonons in Molecular Junctions with Nanoscopic Thermal Baths. Journal of Physical Chemistry C, 2019, 123, 9680-9687.	1.5	7
93	Time-dependent framework for energy and charge currents in nanoscale systems. Chemical Physics, 2018, 514, 176-182.	0.9	6
94	Exploring the similarity of single-layer covalent organic frameworks using electronic structure calculations. RSC Advances, 2022, 12, 12283-12291.	1.7	6
95	Surface-Phonon-Induced Rotational Dissipation for Nanoscale Solid-State Gears. Physical Review Applied, 2021, 15, .	1.5	5
96	An Atomistic Study of the Thermoelectric Signatures of CNT Peapods. Journal of Physical Chemistry C, 2021, 125, 13721-13731.	1.5	5
97	The formation of nanopipes caused by donor impurities in GaN: A theoretical study for the case of oxygen. Philosophical Magazine Letters, 1999, 79, 147-152.	0.5	4
98	Photoassisted transport in silicon dangling bond wires. Applied Physics Letters, 2015, 107, 203109.	1.5	4
99	Modeling of Solvent Effects in the Electrical Response of π -Stacked Molecular Junctions. Journal of Physical Chemistry C, 2015, 119, 20201-20209.	1.5	4
100	Self-Assembled Two-Dimensional Supramolecular Networks Characterized by Scanning Tunneling Microscopy and Spectroscopy in Air and under Vacuum. Langmuir, 2018, 34, 7698-7707.	1.6	4
101	Exploring the organic-inorganic interface in biosilica: atomistic modeling of polyamine and silica precursors aggregation behavior. BMC Materials, 2020, 2, .	6.8	4
102	DNA Conduction: The Issue of Static Disorder, Dynamic Fluctuations and Environmental Effects. , 2006, , 433-464.		3
103	Atomistic Framework for Time-Dependent Thermal Transport. Journal of Physical Chemistry C, 2018, 122, 21062-21068.	1.5	3
104	A nanographene disk rotating a single molecule gear on a Cu(111) surface. Nanotechnology, 2022, 33, 175701.	1.3	3
105	Stability and Reconstruction of, β -SiC (100) Surfaces. Materials Research Society Symposia Proceedings, 1996, 423, 427.	0.1	2
106	Spin-Dependent Effects in Helical Molecular Systems with Rashba-Like Spin-Orbit Interaction. Acta Physica Polonica A, 2015, 127, 185-191.	0.2	2
107	Mechanical Transmission of Rotation for Molecule Gears and Solid-State Gears. Advances in Atom and Single Molecule Machines, 2020, , 165-180.	0.0	2
108	The influence of structural instabilities and non-linear electron-phonon coupling on the isotope effect. Physica C: Superconductivity and Its Applications, 1994, 221, 363-386.	0.6	1

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109	Manifestation of electrode surface states in molecular conduction. Macromolecular Symposia, 2004, 212, 103-112.	0.4	1
110	Vibrational heating in single-molecule switches: an energy-dependent density-of-states approach. Journal of Physics Condensed Matter, 2012, 24, 394003.	0.7	1
111	Exploring the write-in process in molecular quantum cellular automata: a combined modeling and first-principle approach. Journal of Physics Condensed Matter, 2019, 31, 405502.	0.7	1
112	Mapping Conformational Changes in a Self-Assembled Two-Dimensional Molecular Network by Statistical Analysis of Conductance Images. Physical Review Applied, 2019, 11, .	1.5	1
113	Continuum modelling of structure formation of biosilica patterns in diatoms. BMC Materials, 2020, 2, .	6.8	1
114	Nanoscale Phononic Analog of the Ranque-Hilsch Vortex Tube. Physical Review Applied, 2021, 15, .	1.5	1
115	Effect of lubricants on the rotational transmission between solid-state gears. Beilstein Journal of Nanotechnology, 2022, 13, 54-62.	1.5	1
116	Conductance of molecular wires: coherent and incoherent transport (Invited Paper). , 2005, 5838, 182.		0
117	Spin transport in helical biological systems. , 2014, , .		0
118	Nanoscale Molecular Automata: From Materials to Architectures. Natural Computing Series, 2018, , 319-337.	2.2	0
119	The role of structural symmetry on proton tautomerization: A DFTB/Meta-Dynamics computational study. Chemical Physics, 2021, 548, 111222.	0.9	0