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	Effect of lubricants on the rotational transmission between solid-state gears. Beilstein Journal of Nanotechnology, 2022, 13, 54-62.	1.5	1
2	A nanographene disk rotating a single molecule gear on a Cu(111) surface. Nanotechnology, 2022, 33, 175701.	1.3	3
3	A Chirality-Based Quantum Leap. ACS Nano, 2022, 16, 4989-5035.	7.3	74
4	Exploring the similarity of single-layer covalent organic frameworks using electronic structure calculations. RSC Advances, 2022, 12, 12283-12291.	1.7	6
5	The contribution of intermolecular spin interactions to the London dispersion forces between chiral molecules. Journal of Chemical Physics, 2022, 156, .	1.2	9
6	Surface-Phonon-Induced Rotational Dissipation for Nanoscale Solid-State Gears. Physical Review Applied, 2021, 15, .	1.5	5
7	Nanoscale Phononic Analog of the Ranque-Hilsch Vortex Tube. Physical Review Applied, 2021, 15, .	1.5	1
8	An Atomistic Study of the Thermoelectric Signatures of CNT Peapods. Journal of Physical Chemistry C, 2021, 125, 13721-13731.	1.5	5
9	The role of structural symmetry on proton tautomerization: A DFTB/Meta-Dynamics computational study. Chemical Physics, 2021, 548, 111222.	0.9	0
10	A zinc selective oxytocin based biosensor. Journal of Materials Chemistry B, 2020, 8, 155-160.	2.9	11
11	Spin-Polarized Electron Transmission in DNA-Like Systems. Biomolecules, 2020, 10, 49.	1.8	10
12	Role of Exchange Interactions in the Magnetic Response and Intermolecular Recognition of Chiral Molecules. Nano Letters, 2020, 20, 7077-7086.	4.5	35
13	Interactions of Long-Chain Polyamines with Silica Studied by Molecular Dynamics Simulations and Solid-State NMR Spectroscopy. Langmuir, 2020, 36, 11600-11609.	1.6	9
14	Continuum modelling of structure formation of biosilica patterns in diatoms. BMC Materials, 2020, 2, .	6.8	1
15	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
16	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
17	Mechanical Transmission of Rotational Motion between Molecular-Scale Gears. Physical Review Applied, 2020, 13, .	1.5	13
18	Exploring the organicâ€“inorganic interface in biosilica: atomistic modeling of polyamine and silica precursors aggregation behavior. BMC Materials, 2020, 2, .	6.8	4

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19	Understanding the UV luminescence of zinc germanate: The role of native defects. Acta Materialia, 2020, 196, 626-634.	3.8	12
20	Mechanical Transmission of Rotation for Molecule Gears and Solid-State Gears. Advances in Atom and Single Molecule Machines, 2020, , 165-180.	0.0	2
21	Green function, quasi-classical Langevin and Kuboâ€“Greenwood methods in quantum thermal transport. Journal of Physics Condensed Matter, 2019, 31, 273003.	0.7	15
22	Quantum Phonon Transport in Nanomaterials: Combining Atomistic with Non-Equilibrium Greenâ€™s Function Techniques. Entropy, 2019, 21, 735.	1.1	12
23	Direct Assembly and Metal-Ion Binding Properties of Oxytocin Monolayer on Gold Surfaces. Langmuir, 2019, 35, 11114-11122.	1.6	8
24	Chirality-Induced Spin Selectivity in a Coarse-Grained Tight-Binding Model for Helicene. Journal of Physical Chemistry C, 2019, 123, 27230-27241.	1.5	44
25	ITO Work Function Tunability by Polarizable Chromophore Monolayers. Langmuir, 2019, 35, 2997-3004.	1.6	12
26	Doping engineering of thermoelectric transport in BNC heteronanotubes. Physical Chemistry Chemical Physics, 2019, 21, 1904-1911.	1.3	10
27	Current-induced rotations of molecular gears. Journal of Physics Communications, 2019, 3, 025011.	0.5	12
28	Exploring the write-in process in molecular quantum cellular automata: a combined modelingand first-principle approach. Journal of Physics Condensed Matter, 2019, 31, 405502.	0.7	1
29	Impact of device geometry on electron and phonon transport in graphene nanorings. Physical Review B, 2019, 99, .	1.1	7
30	Electron Transport through Self-Assembled Monolayers of Tripeptides. Journal of Physical Chemistry C, 2019, 123, 9600-9608.	1.5	13
31	Selective Transmission of Phonons in Molecular Junctions with Nanoscopic Thermal Baths. Journal of Physical Chemistry C, 2019, 123, 9680-9687.	1.5	7
32	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
33	Thermal bridging of graphene nanosheets via covalent molecular junctions: A non-equilibrium Greenâ€™s functionsâ€“density functional tight-binding study. Nano Research, 2019, 12, 791-799.	5.8	29
34	Chirality-Dependent Electron Spin Filtering by Molecular Monolayers of Helicenes. Journal of Physical Chemistry Letters, 2018, 9, 2025-2030.	2.1	154
35	Time-dependent framework for energy and charge currents in nanoscale systems. Chemical Physics, 2018, 514, 176-182.	0.9	6
36	Firstâ€Principleâ€Based Phonon Transport Properties of Nanoscale Graphene Grain Boundaries. Advanced Science, 2018, 5, 1700365.	5.6	17

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37	Diversification of Device Platforms by Molecular Layers: Hybrid Sensing Platforms, Monolayer Doping, and Modeling. Langmuir, 2018, 34, 14103-14123.	1.6	10
38	Polymerization driven monomer passage through monolayer chemical vapour deposition graphene. Nature Communications, 2018, 9, 4051.	5.8	20
39	Thermal Decoherence and Disorder Effects on Chiral-Induced Spin Selectivity. Journal of Physical Chemistry Letters, 2018, 9, 5753-5758.	2.1	28
40	Enhanced Magnetoresistance in Chiral Molecular Junctions. Journal of Physical Chemistry Letters, 2018, 9, 5453-5459.	2.1	69
41	Nanoscale Molecular Automata: From Materials to Architectures. Natural Computing Series, 2018, , 319-337.	2.2	0
42	Atomistic Framework for Time-Dependent Thermal Transport. Journal of Physical Chemistry C, 2018, 122, 21062-21068.	1.5	3
43	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
44	Spinâ€“orbit coupling in nearly metallic chiral carbon nanotubes: a density-functional based study. Physical Chemistry Chemical Physics, 2017, 19, 8848-8853.	1.3	10
45	Doping of graphene induced by boron/silicon substrate. Nanotechnology, 2017, 28, 215701.	1.3	11
46	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
47	Lightâ€induced Contraction/Expansion of 1D Photoswitchable Metallopolymer Monitored at the Solidâ€“Liquid Interface. Small, 2017, 13, 1701790.	5.2	18
48	Enhancement of thermal transport properties of asymmetric Graphene/hBN nanoribbon heterojunctions by substrate engineering. Carbon, 2017, 124, 642-650.	5.4	27
49	Copper Induced Conformational Changes of Tripeptide Monolayer Based Impedimetric Biosensor. Scientific Reports, 2017, 7, 9498.	1.6	20
50	In-Situ Stretching Patterned Graphene Nanoribbons in the Transmission Electron Microscope. Scientific Reports, 2017, 7, 211.	1.6	26
51	Molecular and Ionic Dipole Effects on the Electronic Properties of Si-/SiO₂-Grafted Alkylamine Monolayers. ACS Applied Materials & Interfaces, 2017, 9, 44873-44879.	4.0	10
52	Coherent spin dynamics in a helical arrangement of molecular dipoles. AIMS Materials Science, 2017, 4, 1052-1061.	0.7	8
53	Anisotropic Thermoelectric Response in Two-Dimensional Puckered Structures. Journal of Physical Chemistry C, 2016, 120, 18841-18849.	1.5	84
54	Discrete polygonal supramolecular architectures of isocytosine-based Pt(<scp>ii</scp>) complexes at the solution/graphite interface. Chemical Communications, 2016, 52, 11163-11166.	2.2	8

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55	Probing Silicaâ€“Biomolecule Interactions by Solid-State NMR and Molecular Dynamics Simulations. Langmuir, 2016, 32, 11698-11705.	1.6	13
56	Atomically Precise Prediction of 2D Selfâ€Assembly of Weakly Bonded Nanostructures: STM Insight into Concentrationâ€Dependent Architectures. Small, 2016, 12, 343-350.	5.2	33
57	Molecular design driving tetraporphyrin self-assembly on graphite: a joint STM, electrochemical and computational study. Nanoscale, 2016, 8, 13678-13686.	2.8	19
58	Quantum interference based Boolean gates in dangling bond loops on Si(100):H surfaces. Scientific Reports, 2015, 5, 14136.	1.6	11
59	Photoassisted transport in silicon dangling bond wires. Applied Physics Letters, 2015, 107, 203109.	1.5	4
60	Engineering thermal rectification in MoS₂nanoribbons: a non-equilibrium molecular dynamics study. RSC Advances, 2015, 5, 54345-54351.	1.7	16
61	Contact effects and quantum interference in engineered dangling bond loops on silicon surfaces. Nanoscale, 2015, 7, 13967-13973.	2.8	8
62	Spin-Dependent Effects in Helical Molecular Systems with Rashba-Like Spin-Orbit Interaction. Acta Physica Polonica A, 2015, 127, 185-191.	0.2	2
63	Interplay between Mechanical and Electronic Degrees of Freedom in Ï€-Stacked Molecular Junctions: From Single Molecules to Mesoscopic Nanoparticle Networks. Journal of Physical Chemistry C, 2015, 119, 6344-6355.	1.5	11
64	Guanosine-based hydrogen-bonded 2D scaffolds: metal-free formation of G-quartet and G-ribbon architectures at the solid/liquid interface. Chemical Communications, 2015, 51, 11677-11680.	2.2	38
65	Modeling of Solvent Effects in the Electrical Response of Ï€-Stacked Molecular Junctions. Journal of Physical Chemistry C, 2015, 119, 20201-20209.	1.5	4
66	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
67	Thermoelectric properties of functionalized graphene grain boundaries. Journal of Self-Assembly and Molecular Electronics (SAME), 2015, 2015, 1-20.	0.0	13
68	Spin transport in helical biological systems. , 2014, , .		0
69	Contact effects in spin transport along double-helical molecules. Physical Review B, 2014, 89, .	1.1	46
70	Structural distortions in molecular-based quantum cellular automata: a minimal model based study. Physical Chemistry Chemical Physics, 2014, 16, 17777-17785.	1.3	7
71	A parabolic model to control quantum interference in T-shaped molecular junctions. Physical Chemistry Chemical Physics, 2013, 15, 13951.	1.3	25
72	Reverse breakdown behavior in organic pin-diodes comprising C60 and pentacene: Experiment and theory. Organic Electronics, 2013, 14, 193-199.	1.4	15

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73	Modeling charge transport in DNA using multiâ€scale methods. Physica Status Solidi (B): Basic Research, 2013, 250, 2277-2287.	0.7	26
74	Dynamic and Electronic Transport Properties of DNA Translocation through Graphene Nanopores. Nano Letters, 2013, 13, 1969-1976.	4.5	115
75	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
76	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
77	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
78	Vibrational heating in single-molecule switches: an energy-dependent density-of-states approach. Journal of Physics Condensed Matter, 2012, 24, 394003.	0.7	1
79	Spin-selective transport through helical molecular systems. Physical Review B, 2012, 85, .	1.1	194
80	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
81	Spin Specific Electron Conduction through DNA Oligomers. Nano Letters, 2011, 11, 4652-4655.	4.5	323
82	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
83	Heat transport and thermal rectification in molecular junctions: A minimal model approach. Physical Review B, 2011, 84, .	1.1	7
84	Engineering the figure of merit and thermopower in single-molecule devices connected to semiconducting electrodes. Physical Review B, 2010, 81, .	1.1	91
85	Organic Zener Diodes: Tunneling across the Gap in Organic Semiconductor Materials. Nano Letters, 2010, 10, 4929-4934.	4.5	64
86	Structural fluctuations and quantum transport through DNA molecular wires: a combined molecular dynamics and model Hamiltonian approach. New Journal of Physics, 2010, 12, 023022.	1.2	53
87	Charge migration through DNA molecules in the presence of mismatches. Physical Review B, 2010, 82, .	1.1	18
88	Distance-dependent coherent charge transport in DNA: crossover from tunneling to free propagation. Journal of Biophysical Chemistry, 2010, 01, 77-85.	0.1	16
89	Charge Transport through Biomolecular Wires in a Solvent: Bridging Molecular Dynamics and Model Hamiltonian Approaches. Physical Review Letters, 2009, 102, 208102.	2.9	80
90	SCREW MOTION OF DNA DUPLEX DURING TRANSLOCATION THROUGH PORE I: INTRODUCTION OF THE COARSE-GRAINED MODEL. Biophysical Reviews and Letters, 2009, 04, 209-230.	0.9	7

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91	Tuning the conductance of a molecular switch. Nature Nanotechnology, 2007, 2, 176-179.	15.6	188
92	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
93	DNA Conduction: The Issue of Static Disorder, Dynamic Fluctuations and Environmental Effects. , 2006, , 433-464.		3
94	Conductance of molecular wires: coherent and incoherent transport (Invited Paper). , 2005, 5838, 182.		0
95	Vibrational effects in the linear conductance of carbon nanotubes. Europhysics Letters, 2005, 71, 438-444.	0.7	38
96	Quantum Transport through a DNA Wire in a Dissipative Environment. Nano Letters, 2005, 5, 1093-1097.	4.5	68
97	Dissipative effects in the electronic transport through DNA molecular wires. Physical Review B, 2005, 71, .	1.1	59
98	Giant magnetoresistance of multiwall carbon nanotubes: Modeling the tube/ferromagnetic-electrode burying contact. Physical Review B, 2004, 69, .	1.1	27
99	Incoherent Electronâ^'Phonon Scattering in Octanethiols. Nano Letters, 2004, 4, 2109-2114.	4.5	106
100	Manifestation of electrode surface states in molecular conduction. Macromolecular Symposia, 2004, 212, 103-112.	0.4	1
101	Conductance Properties of Stilbenoid Molecules. ChemPhysChem, 2003, 4, 1252-1256.	1.0	15
102	Conductance of a molecular junction mediated by unconventional metal-induced gap states. Europhysics Letters, 2003, 62, 90-96.	0.7	23
103	Electronic transport through occupied and unoccupied states of an organic molecule on Au: Experiment and theory. Physical Review B, 2002, 65, .	1.1	32
104	Theory of an all-carbon molecular switch. Physical Review B, 2002, 65, .	1.1	81
105	Conductance Calculations for Real Systems on the Nanoscale. ChemPhysChem, 2002, 3, 650.	1.0	7
106	Fullerene based devices for molecular electronics. Physica E: Low-Dimensional Systems and Nanostructures, 2002, 12, 749-752.	1.3	18
107	Electrical transport properties of small sodium clusters. Physical Review A, 2001, 64, .	1.0	22
108	Observation of â€œStickâ€•and â€œHandleâ€•Intermediates along the Fullerene Road. Physical Review Letters, 2000, 84, 2421-2424.	2.9	52

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109	Reconstructions of the Si-terminated (100) surface inÎ²â^'SiC: A theoretical study. Physical Review B, 1999, 60, 1771-1776.	1.1	20
110	Stoichiometric and non-stoichiometric (101Ì„0) and (112Ì„0) surfaces in 2Hâ€“SiC: a theoretical study. Solid State Communications, 1999, 111, 459-464.	0.9	66
111	Interaction of Oxygen with Threading Dislocations in GaN. Physica Status Solidi A, 1999, 171, 167-173.	1.7	36
112	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
113	Ball-and-Chain Dimers from a Hot Fullerene Plasma. Journal of Physical Chemistry A, 1999, 103, 5275-5284.	1.1	37
114	A theoretical study of O chemisorption on GaN (0001)/(0001Ì„) surfaces. Solid State Communications, 1998, 108, 953-958.	0.9	18
115	Effect of oxygen on the growth of (101Ì„0) GaN surfaces: The formation of nanopipes. Applied Physics Letters, 1998, 73, 3530-3532.	1.5	66
116	Stability of silicon carbide structures: from clusters to solid surfaces. Journal of Materials Chemistry, 1996, 6, 1657-1663.	6.7	22
117	Stability and Reconstruction of, Î²-SiC (100) Surfaces. Materials Research Society Symposia Proceedings, 1996, 423, 427.	0.1	2
118	Ionization energies and Coulomb explosion of highly charged C60. Physics Letters, Section A: General, Atomic and Solid State Physics, 1996, 211, 357-362.	0.9	48
119	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