

LuÃ-s Gc Rego

List of Publications by Year in descending order

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59
papers

2,441
citations

331259

21
h-index

197535

49
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59
all docs

59
docs citations

59
times ranked

2353
citing authors

#	ARTICLE	IF	CITATIONS
1	Quantized Thermal Conductance of Dielectric Quantum Wires. <i>Physical Review Letters</i> , 1998, 81, 232-235.	2.9	618
2	Quantum Dynamics Simulations of Interfacial Electron Transfer in Sensitized TiO ₂ Semiconductors. <i>Journal of the American Chemical Society</i> , 2003, 125, 7989-7997.	6.6	368
3	Influence of Thermal Fluctuations on Interfacial Electron Transfer in Functionalized TiO ₂ Semiconductors. <i>Journal of the American Chemical Society</i> , 2005, 127, 18234-18242.	6.6	196
4	Quantum conductance in silver nanowires: Correlation between atomic structure and transport properties. <i>Physical Review B</i> , 2002, 65, .	1.1	157
5	Surface Effects and Adsorption of Methoxy Anchors on Hybrid Lead Iodide Perovskites: Insights for Spiro-MeOTAD Attachment. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26947-26954.	1.5	115
6	Indication of Unusual Pentagonal Structures in Atomic-Size Cu Nanowires. <i>Physical Review Letters</i> , 2004, 93, 126103.	2.9	105
7	Fractional exclusion statistics and the universal quantum of thermal conductance: A unifying approach. <i>Physical Review B</i> , 1999, 59, 13080-13086.	1.1	88
8	What Makes Hydroxamate a Promising Anchoring Group in Dye-Sensitized Solar Cells? Insights from Theoretical Investigation. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3992-3999.	2.1	61
9	Crucial Role of Nuclear Dynamics for Electron Injection in a Dye-Semiconductor Complex. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2393-2398.	2.1	49
10	Model study of coherent quantum dynamics of hole states in functionalized semiconductor nanostructures. <i>Journal of Chemical Physics</i> , 2005, 122, 154709.	1.2	43
11	Subpicosecond Dynamics of Metal-to-Ligand Charge-Transfer Excited States in Solvated [Ru(bpy) ₃] ²⁺ Complexes. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15617-15626.	1.5	39
12	Coupled Electron-Hole Quantum Dynamics on Dye-Sensitized TiO ₂ Semiconductors. <i>Journal of Physical Chemistry C</i> , 2012, 116, 21169-21178.	1.5	38
13	Visible Light Sensitization of TiO ₂ Surfaces with Alq ₃ Complexes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 1317-1325.	1.5	37
14	Intramolecular Polarization Induces Electron-Hole Charge Separation in Light-Harvesting Molecular Triads. <i>Journal of Physical Chemistry C</i> , 2014, 118, 126-134.	1.5	37
15	Study of Redox Species and Oxygen Vacancy Defects at TiO ₂ Electrolyte Interfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19433-19442.	1.5	36
16	Interacting valence holes in p-type SiGe quantum disks in a magnetic field. <i>Physical Review B</i> , 1997, 55, 15694-15700.	1.1	35
17	Coherent Control of Quantum Dynamics with Sequences of Unitary Phase-Kick Pulses. <i>Annual Review of Physical Chemistry</i> , 2009, 60, 293-320.	4.8	35
18	Vibronic and Coherent Effects on Interfacial Electron Transfer Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4927-4935.	2.1	34

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19	Ultrafast Interfacial Charge-Transfer Dynamics in a Donor-Å-Acceptor Chromophore Sensitized TiO ₂ Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4824-4835.	1.5	33
20	Magnetic properties of nanoparticles in the Bethe-Peierls approximation. <i>Physical Review B</i> , 2001, 64, .	1.1	27
21	Theoretical investigation of the adsorption, IR, and electron injection of hydroxamate anchor at the TiO ₂ anatase (1 0 1) surface. <i>RSC Advances</i> , 2014, 4, 19690-19693.	1.7	26
22	A Nonadiabatic Excited State Molecular Mechanics/Extended HÃ¼ckel Ehrenfest Method. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27688-27698.	1.5	22
23	Quantum chaos in nanoelectromechanical systems. <i>Physical Review B</i> , 2006, 73, .	1.1	16
24	Charge Generation in Organic Solar Cells: Interplay of Quantum Dynamics, Decoherence, and Recombination. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23276-23286.	1.5	15
25	Vibronic Effects in the Ultrafast Interfacial Electron Transfer of Perylene-Sensitized TiO ₂ Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12599-12607.	1.5	15
26	Coherent control of tunnelling dynamics in functionalized semiconductor nanostructures: a quantum-control scenario based on stochastic unitary pulses. <i>Journal of Modern Optics</i> , 2006, 53, 2519-2532.	0.6	13
27	Charge Transfer Driven Structural Relaxation in a Push-Pull Azobenzene Dye-Semiconductor Complex. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5926-5933.	2.1	12
28	Modulating the Photoisomerization Mechanism of Semiconductor-Bound Azobenzene-Functionalized Compounds. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5692-5698.	1.5	12
29	Diffusion, reaction and forced convection in electrochemical cells. <i>Journal of Electroanalytical Chemistry</i> , 2009, 628, 21-26.	1.9	11
30	Coupled quantum-classical method for long range charge transfer: relevance of the nuclear motion to the quantum electron dynamics. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 134206.	0.7	11
31	Quantum Dynamics Simulations of Excited State Energy Transfer in a Zinc-Free-Base Porphyrin Dyad. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8075-8084.	1.1	11
32	Chirality-Induced Propagation Velocity Asymmetry. <i>Nano Letters</i> , 2021, 21, 8190-8196.	4.5	10
33	Chapter 4. Modelling electron quantum dynamics in large molecular systems. <i>Chemical Modelling</i> , 2013, , 102-126.	0.2	10
34	Electronic-Vibrational Coupling and Electron Transfer. <i>Journal of Physical Chemistry C</i> , 2019, 123, 23760-23772.	1.5	9
35	Anomalous quantum chaotic behaviour in suspended electromechanical nanostructures. <i>Journal of Physics A</i> , 2005, 38, L639-L645.	1.6	8
36	Coherent optical control of electronic excitations in functionalized semiconductor nanostructures. <i>Quantum Information and Computation</i> , 2005, 5, 318-334.	0.1	8

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37	Interface roughness localization in quantum wells and quantum wires. <i>Physical Review B</i> , 1998, 58, 9876-9880.	1.1	7
38	Rego and Kirczenow Reply. <i>Physical Review Letters</i> , 1998, 81, 5038-5038.	2.9	7
39	Synthesis and Properties of Perylene-Bridge-Anchored Chromophoric Compounds. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6330-6343.	1.1	7
40	The two-dimensional D [∞] complex in intense AC and strong magnetic fields. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 1998, 3, 198-204.	1.3	6
41	Heat capacity of suspended phonon cavities. <i>Physical Review B</i> , 2007, 75, .	1.1	6
42	Decoherence effects on quantum control by reverse optimized pulse sequences. <i>Physical Review A</i> , 2012, 86, .	1.0	6
43	Multi-charged acceptor centers in p-doped Si/Si ^{1-λ} Gex/Si quantum wells in the presence of a magnetic field. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 1998, 2, 785-788.	1.3	5
44	Thermal Transport in the Quantum Regime. <i>Physica Status Solidi A</i> , 2001, 187, 239-251.	1.7	5
45	Inferring Protonation States of Hydroxamate Adsorbates on TiO ₂ Surfaces. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11985-11990.	1.5	5
46	Mechanism for LO-phonon temperature overshoot in GaAs. <i>Physical Review B</i> , 1994, 49, 7257-7261.	1.1	4
47	Superconducting Qubits as Mechanical Quantum Engines. <i>Physical Review Letters</i> , 2017, 119, 090601.	2.9	4
48	Conformational and Binding Effects on Interfacial Electron Transfer from Dual-Linker Sensitizers. <i>Journal of Physical Chemistry C</i> , 2021, 125, 8667-8676.	1.5	4
49	Electrostatic mechanism for cooling semiconductor heterostructures. <i>Applied Physics Letters</i> , 1999, 75, 2262-2264.	1.5	3
50	Multiple unitary-pulses for coherent-control of tunnelling and decoherence. <i>Journal of Modern Optics</i> , 2007, 54, 2617-2627.	0.6	3
51	Comment on "Wave-scattering formalism for thermal conductance in thin wires with surface disorder". <i>Physical Review B</i> , 2010, 81, .	1.1	2
52	Energetics of the charge generation in organic donor-acceptor interfaces. <i>Journal of Chemical Physics</i> , 2022, 156, 024104.	1.2	2
53	Electronic structure of holes in modulation doped p-Si ^{1-λ} Gex/Si strained quantum wells in a magnetic field. <i>Solid State Communications</i> , 1998, 105, 139-144.	0.9	1
54	Confinement versus localization for quantum wells and quantum wires in a self-assembled structure. <i>Superlattices and Microstructures</i> , 1999, 25, 137-141.	1.4	1

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55	A new principle for electronic cooling of mesoscopic systems. Physica E: Low-Dimensional Systems and Nanostructures, 2000, 6, 840-843.	1.3	1
56	Thermodynamics of half-filled Landau levels: A study of the composite fermion mass. Physical Review B, 2000, 62, 1544-1547.	1.1	1
57	Effect of intermittent convection movements on voltammogram and current transients. Journal of Chemical Physics, 2008, 128, 054501.	1.2	1
58	Model calculation of the femtosecond carrier dynamics in Al _{0.48} Ga _{0.52} As. Journal of Applied Physics, 1994, 76, 3749-3753.	1.1	0
59	Force field parameters for large-scale computational modeling of sensitized TiO ₂ surfaces. , 2006, , .		0