Iain Grace

List of Publications by Year in descending order

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236612 243296 2,017 54 25 44 citations h-index g-index papers 57 57 57 2039 all docs docs citations times ranked citing authors

#	Article	IF	CITATIONS
1	Quantum interference dependence on molecular configurations for cross-conjugated systems in single-molecule junctions. Molecular Systems Design and Engineering, 2022, 7, 1287-1293.	1.7	5
2	Assembly, structure and thermoelectric properties of 1,1′-dialkynylferrocene  hinges'. Chemical Science, 2022, 13, 8380-8387.	3.7	8
3	Interference Controls Conductance in Phthalocyanine Molecular Junctions. Journal of Physical Chemistry C, 2021, 125, 15035-15043.	1.5	7
4	Molecular-scale thermoelectricity: as simple as â€~ABC'. Nanoscale Advances, 2020, 2, 5329-5334.	2.2	16
5	Solvent-molecule interaction induced gating of charge transport through single-molecule junctions. Science Bulletin, 2020, 65, 944-950.	4.3	16
6	Redox Control of Charge Transport in Vertical Ferrocene Molecular Tunnel Junctions. CheM, 2020, 6, 1172-1182.	5.8	40
7	Connectivity dependent thermopower of bridged biphenyl molecules in single-molecule junctions. Nanoscale, 2020, 12, 14682-14688.	2.8	13
8	Scale-Up of Room-Temperature Constructive Quantum Interference from Single Molecules to Self-Assembled Molecular-Electronic Films. Journal of the American Chemical Society, 2020, 142, 8555-8560.	6.6	34
9	Electrical molecular switch addressed by chemical stimuli. Nanoscale, 2020, 12, 10127-10139.	2.8	14
10	Cross-conjugation increases the conductance of <i>meta</i> -connected fluorenones. Nanoscale, 2019, 11, 13720-13724.	2.8	25
11	Synthetic Control of Quantum Interference by Regulating Charge on a Single Atom in Heteroaromatic Molecular Junctions. Journal of Physical Chemistry Letters, 2019, 10, 6419-6424.	2.1	25
12	Charge transfer complexation boosts molecular conductance through Fermi level pinning. Chemical Science, 2019, 10, 2396-2403.	3.7	47
13	Self-Assembled Molecular-Electronic Films Controlled by Room Temperature Quantum Interference. CheM, 2019, 5, 474-484.	5.8	45
14	Gateway state-mediated, long-range tunnelling in molecular wires. Nanoscale, 2018, 10, 3060-3067.	2.8	25
15	Detecting Mechanochemical Atropisomerization within an STM Break Junction. Journal of the American Chemical Society, 2018, 140, 710-718.	6.6	38
16	Toward High Thermoelectric Performance of Thiophene and Ethylenedioxythiophene (EDOT) Molecular Wires. Advanced Functional Materials, 2018, 28, 1703135.	7.8	42
17	Cross-plane conductance through a graphene/molecular monolayer/Au sandwich. Nanoscale, 2018, 10, 19791-19798.	2.8	12
18	Quantum interference mediated vertical molecular tunneling transistors. Science Advances, 2018, 4, eaat8237.	4.7	64

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19	Bias-Driven Conductance Increase with Length in Porphyrin Tapes. Journal of the American Chemical Society, 2018, 140, 12877-12883.	6.6	84
20	Unconventional Single-Molecule Conductance Behavior for a New Heterocyclic Anchoring Group: Pyrazolyl. Journal of Physical Chemistry Letters, 2018, 9, 5364-5372.	2.1	33
21	Oscillating Seebeck coefficients in π-stacked molecular junctions. RSC Advances, 2018, 8, 24711-24715.	1.7	20
22	Soft versus hard junction formation for \hat{l}_{\pm} -terthiophene molecular wires and their charge transfer complexes. Journal of Chemical Physics, 2017, 146, .	1.2	6
23	Suppression of Phonon Transport in Molecular Christmas Trees. ChemPhysChem, 2017, 18, 1234-1241.	1.0	27
24	Connectivity dependence of Fano resonances in single molecules. Physical Chemistry Chemical Physics, 2017, 19, 6416-6421.	1.3	22
25	Discriminating single-molecule sensing by crown-ether-based molecular junctions. Journal of Chemical Physics, 2017, 146, 064704.	1.2	14
26	The single-molecule electrical conductance of a rotaxane-hexayne supramolecular assembly. Nanoscale, 2017, 9, 355-361.	2.8	47
27	Electrochemical control of the single molecule conductance of a conjugated bis(pyrrolo)tetrathiafulvalene based molecular switch. Chemical Science, 2017, 8, 6123-6130.	3.7	31
28	Sideâ€Groupâ€Mediated Mechanical Conductance Switching in Molecular Junctions. Angewandte Chemie - International Edition, 2017, 56, 15378-15382.	7.2	74
29	Sideâ€Groupâ€Mediated Mechanical Conductance Switching in Molecular Junctions. Angewandte Chemie, 2017, 129, 15580-15584.	1.6	12
30	Tuning the electrical conductance of metalloporphyrin supramolecular wires. Scientific Reports, 2016, 6, 37352.	1.6	27
31	Charge transport through dicarboxylic-acid-terminated alkanes bound to graphene–gold nanogap electrodes. Nanoscale, 2016, 8, 14507-14513.	2.8	16
32	Molecular design and control of fullerene-based bi-thermoelectric materials. Nature Materials, 2016, 15, 289-293.	13.3	132
33	Tuning the thermoelectric properties of metallo-porphyrins. Nanoscale, 2016, 8, 2428-2433.	2.8	33
34	Exploiting the extended π-system of perylene bisimide for label-free single-molecule sensing. Journal of Materials Chemistry C, 2015, 3, 2101-2106.	2.7	16
35	Increasing the thermopower of crown-ether-bridged anthraquinones. Nanoscale, 2015, 7, 17338-17342.	2.8	20
36	Gating of single molecule junction conductance by charge transfer complex formation. Nanoscale, 2015, 7, 18949-18955.	2.8	41

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37	Thermoelectric performance of various benzo-difuran wires. Journal of Chemical Physics, 2014, 140, 174711.	1.2	4
38	A Sm(II)-Mediated Cascade Approach to Dibenzoindolo [3,2-b] carbazoles: Synthesis and Evaluation. Organic Letters, 2014, 16, 2292-2295.	2.4	40
39	Extended conjugation in poly(triarylamine)s: synthesis, structure and impact on field-effect mobility. Journal of Materials Chemistry C, 2014, 2, 6520-6528.	2.7	13
40	Triarylamine polymers of bridged phenylenes by (N-heterocyclic carbene)-palladium catalysed C–N coupling. Journal of Materials Chemistry C, 2013, 1, 3327.	2.7	17
41	A Detailed Experimental and Theoretical Study into the Properties of C ₆₀ Dumbbell Junctions. Small, 2013, 9, 3812-3822.	5.2	11
42	Phase Tag-Assisted Synthesis of Benzo[<i>b</i>]carbazole End-Capped Oligothiophenes. Organic Letters, 2012, 14, 5744-5747.	2.4	25
43	Synthesis of Covalently Linked Molecular Bridges between Silicon Electrodes in CMOSâ€Based Arrays of Vertical Si/SiO ₂ /Si Nanogaps. Angewandte Chemie - International Edition, 2011, 50, 8722-8726.	7.2	15
44	Electron transport through ribbonlike molecular wires calculated using density-functional theory and Greenâ \in^{TM} s function formalism. Physical Review B, 2010, 81, .	1.1	15
45	Molecular Bridging of Silicon Nanogaps. ACS Nano, 2010, 4, 7401-7406.	7.3	37
46	Identifying Diversity in Nanoscale Electrical Break Junctions. Journal of the American Chemical Society, 2010, 132, 9157-9164.	6.6	124
47	Environmental Effects on the Single Molecule Conductance of bis(thiahexyl)oligothiophenes. Materials Research Society Symposia Proceedings, 2009, 1154, 1.	0.1	0
48	Conformation dependence of molecular conductance: chemistry versus geometry. Journal of Physics Condensed Matter, 2008, 20, 022203.	0.7	37
49	Synthesis and Properties of Functionalized 4 nm Scale Molecular Wires with Thiolated Termini for Self-Assembly onto Metal Surfaces. Journal of Organic Chemistry, 2008, 73, 4810-4818.	1.7	27
50	Variable contact gap single-molecule conductance determination for a series of conjugated molecular bridges. Journal of Physics Condensed Matter, 2008, 20, 374119.	0.7	49
51	Single-molecule electrical studies on a 7 nm long molecular wire. Chemical Communications, 2006, , 4706.	2.2	56
52	Precision control of single-molecule electrical junctions. Nature Materials, 2006, 5, 995-1002.	13.3	294
53	Control of electron transport through Fano resonances in molecular wires. Physical Review B, 2006, 74, .	1.1	120
54	Controlled Electron Transport Through Single Molecules. , 2006, , .		О