# Iain Grace

List of Publications by Year
in descending order



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|---|---|---|---|
| 54 papers | 2,017 citations | 236925 25 h-index | 243625 44 g-index |
| 57 all docs | 57 docs citations | 57 times ranked | 2039 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Precision control of single-molecule electrical junctions. Nature Materials, 2006, 5, 995-1002. | 27.5 | 294 |
| 2 | Molecular design and control of fullerene-based bi-thermoelectric materials. Nature Materials, 2016, 15, 289-293. | 27.5 | 132 |
| 3 | Identifying Diversity in Nanoscale Electrical Break Junctions. Journal of the American Chemical Society, 2010, 132, 9157-9164. | 13.7 | 124 |
| 4 | Control of electron transport through Fano resonances in molecular wires. Physical Review B, 2006, 74, . | 3.2 | 120 |
| 5 | Bias-Driven Conductance Increase with Length in Porphyrin Tapes. Journal of the American Chemical Society, 2018, 140, 12877-12883. | 13.7 | 84 |
| 6 | Sideâ€Groupâ€Mediated Mechanical Conductance Switching in Molecular Junctions. Angewandte Chemie - International Edition, 2017, 56, 15378-15382. | 13.8 | 74 |
| 7 | Quantum interference mediated vertical molecular tunneling transistors. Science Advances, 2018, 4, eaat8237. | 10.3 | 64 |
| 8 | Single-molecule electrical studies on a 7 nm long molecular wire. Chemical Communications, 2006, , 4706. | 4.1 | 56 |
| 9 | Variable contact gap single-molecule conductance determination for a series of conjugated molecular bridges. Journal of Physics Condensed Matter, 2008, 20, 374119. | 1.8 | 49 |
| 10 | The single-molecule electrical conductance of a rotaxane-hexayne supramolecular assembly. Nanoscale, 2017, 9, 355-361. | 5.6 | 47 |
| 11 | Charge transfer complexation boosts molecular conductance through Fermi level pinning. Chemical Science, 2019, 10, 2396-2403. | 7.4 | 47 |
| 12 | Self-Assembled Molecular-Electronic Films Controlled by Room Temperature Quantum Interference. CheM, 2019, 5, 474-484. | 11.7 | 45 |
| 13 | Toward High Thermoelectric Performance of Thiophene and Ethylenedioxythiophene (EDOT) Molecular Wires. Advanced Functional Materials, 2018, 28, 1703135. | 14.9 | 42 |
| 14 | Gating of single molecule junction conductance by charge transfer complex formation. Nanoscale, 2015, 7, 18949-18955. | 5.6 | 41 |
| 15 | A Sm(II)-Mediated Cascade Approach to Dibenzoindolo[3,2-b]carbazoles: Synthesis and Evaluation. Organic Letters, 2014, 16, 2292-2295. | 4.6 | 40 |
| 16 | Redox Control of Charge Transport in Vertical Ferrocene Molecular Tunnel Junctions. CheM, 2020, 6, 1172-1182. | 11.7 | 40 |
| 17 | Detecting Mechanochemical Atropisomerization within an STM Break Junction. Journal of the American Chemical Society, 2018, 140, 710-718. | 13.7 | 38 |
| 18 | Conformation dependence of molecular conductance: chemistry versus geometry. Journal of Physics Condensed Matter, 2008, 20, 022203. | 1.8 | 37 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Molecular Bridging of Silicon Nanogaps. ACS Nano, 2010, 4, 7401-7406. | 14.6 | 37 |
| 20 | 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. | 13.7 | 34 |
| 21 | Tuning the thermoelectric properties of metallo-porphyrins. Nanoscale, 2016, 8, 2428-2433. | 5.6 | 33 |
| 22 | Unconventional Single-Molecule Conductance Behavior for a New Heterocyclic Anchoring Group: Pyrazolyl. Journal of Physical Chemistry Letters, 2018, 9, 5364-5372. | 4.6 | 33 |
| 23 | Electrochemical control of the single molecule conductance of a conjugated bis(pyrrolo)tetrathiafulvalene based molecular switch. Chemical Science, 2017, 8, 6123-6130. | 7.4 | 31 |
| 24 | 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. | 3.2 | 27 |
| 25 | Tuning the electrical conductance of metalloporphyrin supramolecular wires. Scientific Reports, 2016, 6, 37352. | 3.3 | 27 |
| 26 | Suppression of Phonon Transport in Molecular Christmas Trees. ChemPhysChem, 2017, 18, 1234-1241. | 2.1 | 27 |
| 27 | Phase Tag-Assisted Synthesis of Benzo[b]carbazole End-Capped Oligothiophenes. Organic Letters, 2012, 14, 5744-5747. | 4.6 | 25 |
| 28 | Gateway state-mediated, long-range tunnelling in molecular wires. Nanoscale, 2018, 10, 3060-3067. | 5.6 | 25 |
| 29 | Cross-conjugation increases the conductance of meta-connected fluorenones. Nanoscale, 2019, 11, 13720-13724. | 5.6 | 25 |
| 30 | 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. | 4.6 | 25 |
| 31 | Connectivity dependence of Fano resonances in single molecules. Physical Chemistry Chemical Physics, 2017, 19, 6416-6421. | 2.8 | 22 |
| 32 | Increasing the thermopower of crown-ether-bridged anthraquinones. Nanoscale, 2015, 7, 17338-17342. | 5.6 | 20 |
| 33 | Oscillating Seebeck coefficients in Ï€-stacked molecular junctions. RSC Advances, 2018, 8, 24711-24715. | 3.6 | 20 |
| 34 | Triarylamine polymers of bridged phenylenes by (N-heterocyclic carbene)-palladium catalysed Câ€“N coupling. Journal of Materials Chemistry C, 2013, 1, 3327. | 5.5 | 17 |
| 35 | Exploiting the extended Ï€-system of perylene bisimide for label-free single-molecule sensing. Journal of Materials Chemistry C, 2015, 3, 2101-2106. | 5.5 | 16 |
| 36 | Charge transport through dicarboxylic-acid-terminated alkanes bound to grapheneâ€“gold nanogap electrodes. Nanoscale, 2016, 8, 14507-14513. | 5.6 | 16 |

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|---|---|---|---|
| 37 | Molecular-scale thermoelectricity: as simple as â€˜ABCâ€™. Nanoscale Advances, 2020, 2, 5329-5334. | 4.6 | 16 |
| 38 | Solvent-molecule interaction induced gating of charge transport through single-molecule junctions. Science Bulletin, 2020, 65, 944-950. | 9.0 | 16 |
| 39 | Electron transport through ribbonlike molecular wires calculated using density-functional theory and Greenâ€™s function formalism. Physical Review B, 2010, 81, . | 3.2 | 15 |
| 40 | Synthesis of Covalently Linked Molecular Bridges between Silicon Electrodes in CMOSâ€Based Arrays of Vertical Si/SiO<sub>2</sub>/Si Nanogaps. Angewandte Chemie - International Edition, 2011, 50, 8722-8726. | 13.8 | 15 |
| 41 | Discriminating single-molecule sensing by crown-ether-based molecular junctions. Journal of Chemical Physics, 2017, 146, 064704. | 3.0 | 14 |
| 42 | Electrical molecular switch addressed by chemical stimuli. Nanoscale, 2020, 12, 10127-10139. | 5.6 | 14 |
| 43 | Extended conjugation in poly(triarylamine)s: synthesis, structure and impact on field-effect mobility. Journal of Materials Chemistry C, 2014, 2, 6520-6528. | 5.5 | 13 |
| 44 | Connectivity dependent thermopower of bridged biphenyl molecules in single-molecule junctions. Nanoscale, 2020, 12, 14682-14688. | 5.6 | 13 |
| 45 | Sideâ€Groupâ€Mediated Mechanical Conductance Switching in Molecular Junctions. Angewandte Chemie, 2017, 129, 15580-15584. | 2.0 | 12 |
| 46 | Cross-plane conductance through a graphene/molecular monolayer/Au sandwich. Nanoscale, 2018, 10, 19791-19798. | 5.6 | 12 |
| 47 | A Detailed Experimental and Theoretical Study into the Properties of C<sub>60</sub> Dumbbell Junctions. Small, 2013, 9, 3812-3822. | 10.0 | 11 |
| 48 | Assembly, structure and thermoelectric properties of 1,1â€²-dialkynylferrocene â€˜hingesâ€™. Chemical Science, 2022, 13, 8380-8387. | 7.4 | 8 |
| 49 | Interference Controls Conductance in Phthalocyanine Molecular Junctions. Journal of Physical Chemistry C, 2021, 125, 15035-15043. | 3.1 | 7 |
| 50 | Soft versus hard junction formation for Î±-terthiophene molecular wires and their charge transfer complexes. Journal of Chemical Physics, 2017, 146, . | 3.0 | 6 |
| 51 | Quantum interference dependence on molecular configurations for cross-conjugated systems in single-molecule junctions. Molecular Systems Design and Engineering, 2022, 7, 1287-1293. | 3.4 | 5 |
| 52 | Thermoelectric performance of various benzo-difuran wires. Journal of Chemical Physics, 2014, 140, 174711. | 3.0 | 4 |
| 53 | Controlled Electron Transport Through Single Molecules. , 2006, , . | | 0 |
| 54 | Environmental Effects on the Single Molecule Conductance of bis(thiahexyl)oligothiophenes. Materials Research Society Symposia Proceedings, 2009, 1154, 1. | 0.1 | 0 |