

# Ivan Rungger

## List of Publications by Year in descending order

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Version: 2024-02-01

36  
papers

1,076  
citations

394421

19  
h-index

395702

33  
g-index

37  
all docs

37  
docs citations

37  
times ranked

1463  
citing authors

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | Spin-orbit induced equilibrium spin currents in materials. Physical Review B, 2022, 105, .  | 3.2  | 3         |
| 2  | $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{DFT} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle + \langle \text{mml:mo} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:m} \text{mathvariant="normal"} \rangle \text{Î} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$<br>method for electron correlation effects at transition metal surfaces. Physical Review B, 2022, 105, . | 3.2  | 7         |
| 3  | Pressure-induced electronic transitions in samarium monochalcogenides. Physical Review B, 2022, 105, .  | 3.2  | 2         |
| 4  | Quantum state discrimination using noisy quantum neural networks. Physical Review Research, 2021, 3, .  | 3.6  | 19        |
| 5  | Maximally localized dynamical quantum embedding for solving many-body correlated systems. Nature Computational Science, 2021, 1, 410-420.   | 8.0  | 6         |
| 6  | Evaluating the noise resilience of variational quantum algorithms. Physical Review A, 2021, 104, .  | 2.5  | 25        |
| 7  | Enhanced thermopower in covalent graphite-molecule contacts. Physical Chemistry Chemical Physics, 2020, 22, 1466-1474.  | 2.8  | 1         |
| 8  | Application of conserved thermal-noise energy model to damped resonant behavior in cryogenic current comparators. Review of Scientific Instruments, 2020, 91, 105115.   | 1.3  | 1         |
| 9  | Non-equilibrium Green's Function Methods for Spin Transport and Dynamics. , 2020, , 957-983.  |      | 5         |
| 10 | Performance analysis of a pairwise method for partial inversion of complex block tridiagonal matrices. Concurrency Computation Practice and Experience, 2019, 31, e4918.  | 2.2  | 2         |
| 11 | Robust Organic Radical Molecular Junctions Using Acetylene Terminated Groups for Au Bond Formation. Journal of the American Chemical Society, 2018, 140, 1691-1696.   | 13.7 | 79        |
| 12 | Non-equilibrium Green's Function Methods for Spin Transport and Dynamics. , 2018, , 1-27.   |      | 2         |
| 13 | Predicting the conductance of strongly correlated molecules: the Kondo effect in perchlorotriphenylmethyl/Au junctions. Nanoscale, 2018, 10, 17738-17750.   | 5.6  | 22        |
| 14 | Quantum transport simulation scheme including strong correlations and its application to organic radicals adsorbed on gold. Physical Review B, 2017, 95, .  | 3.2  | 31        |
| 15 | Stable anchoring chemistry for room temperature charge transport through graphite-molecule contacts. Science Advances, 2017, 3, e1602297.   | 10.3 | 23        |
| 16 | Covalent Modification of Highly Ordered Pyrolytic Graphite with a Stable Organic Free Radical by Using Diazonium Chemistry. Chemistry - A European Journal, 2017, 23, 1415-1421.  | 3.3  | 14        |
| 17 | A redox-active radical as an effective nanoelectronic component: stability and electrochemical tunnelling spectroscopy in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 27733-27737.  | 2.8  | 7         |
| 18 | Fundamental gap of molecular crystals via constrained density functional theory. Physical Review B, 2016, 93, .   | 3.2  | 13        |

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 19 | Dynamic spin filtering at the Co/Alq3 interface mediated by weakly coupled second layer molecules. Nature Communications, 2016, 7, 12668.   | 12.8 | 55        |
| 20 | Transmission through correlated $\text{Cu}$ Physical Review B, 2015, 92, .  | 3.2  | 15        |
| 21 | Electronic Transport as a Driver for Self-Interaction-Corrected Methods. Advances in Atomic, Molecular and Optical Physics, 2015, 64, 29-86.  | 2.3  | 7         |
| 22 | The image charge effect and vibron-assisted processes in Coulomb blockade transport: a first principles approach. Nanoscale, 2015, 7, 19231-19240.                                      | 5.6  | 8         |
| 23 | Controlling the Spin Texture of Topological Insulators by Rational Design of Organic Molecules. Nano Letters, 2015, 15, 6022-6029.  | 9.1  | 37        |
| 24 | Ab initio transport across bismuth selenide surface barriers. Physical Review B, 2014, 90, .  | 3.2  | 14        |
| 25 | Stretching of BDT-gold molecular junctions: thiol or thiolate termination?. Nanoscale, 2014, 6, 14495-14507.  | 5.6  | 40        |
| 26 | Structural Origins of Conductance Fluctuations in Gold-Thiolate Molecular Transport Junctions. Journal of Physical Chemistry Letters, 2013, 4, 887-891.                                 | 4.6  | 33        |
| 27 | Constrained-DFT method for accurate energy-level alignment of metal/molecule interfaces. Physical Review B, 2013, 88, .   | 3.2  | 54        |
| 28 | Atomistic simulations of highly conductive molecular transport junctions under realistic conditions. Nanoscale, 2013, 5, 3654.  | 5.6  | 38        |
| 29 | Topological surface states scattering in antimony. Physical Review B, 2012, 86, .   | 3.2  | 21        |
| 30 | First-principles study of high-conductance DNA sequencing with carbon nanotube electrodes. Physical Review B, 2012, 85, .   | 3.2  | 30        |
| 31 | Prediction of large bias-dependent magnetoresistance in all-oxide magnetic tunnel junctions with a ferroelectric barrier. Physical Review B, 2011, 83, .                                | 3.2  | 25        |
| 32 | Current-induced energy barrier suppression for electromigration from first principles. Physical Review B, 2011, 84, .   | 3.2  | 22        |
| 33 | Quantum conductance of a single magnetic atom: An <i>ab initio</i> study. Physical Review B, 2010, 82, .  | 3.2  | 19        |
| 34 | Resonant electronic states and $I$ vs $V$ curves of Fe/MgO/Fe(100) tunnel junctions. Physical Review B, 2009, 79, .   | 3.2  | 57        |
| 35 | <i>Ab initio</i> calculation of the bias-dependent transport properties of $\text{Mn}$ Physical Review B, 2009, 80, .   | 3.2  | 60        |
| 36 | Algorithm for the construction of self-energies for electronic transport calculations based on singularity elimination and singular value decomposition. Physical Review B, 2008, 78, . | 3.2  | 279       |