Ivan Rungger

List of Publications by Year
in descending order

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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	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
2	Robust Organic Radical Molecular Junctions Using Acetylene Terminated Groups for Câ€“Au Bond Formation. Journal of the American Chemical Society, 2018, 140, 1691-1696.	13.7	79
3	Ab initiocalculation of the bias-dependent transport properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mn</mml:mtext></mml:mrow><mml:mrow><mml:mn>12</mml:mn> Physical Review B, 2009, 80, .	3.2	60
4	Resonant electronic states and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>I</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>V</mml:mi></mml:mrow></mml:math>curve of Fe/MgO/Fe(100) tunnel junctions. Physical Review B, 2009, 79, .	3.2	57
5	Dynamic spin filtering at the Co/Alq3 interface mediated by weakly coupled second layer molecules. Nature Communications, 2016, 7, 12668.	12.8	55
6	Constrained-DFT method for accurate energy-level alignment of metal/molecule interfaces. Physical Review B, 2013, 88, .	3.2	54
7	Stretching of BDT-gold molecular junctions: thiol or thiolate termination?. Nanoscale, 2014, 6, 14495-14507.	5.6	40
8	Atomistic simulations of highly conductive molecular transport junctions under realistic conditions. Nanoscale, 2013, 5, 3654.	5.6	38
9	Controlling the Spin Texture of Topological Insulators by Rational Design of Organic Molecules. Nano Letters, 2015, 15, 6022-6029.	9.1	37
10	Structural Origins of Conductance Fluctuations in Goldâ€“Thiolate Molecular Transport Junctions. Journal of Physical Chemistry Letters, 2013, 4, 887-891.	4.6	33
11	Quantum transport simulation scheme including strong correlations and its application to organic radicals adsorbed on gold. Physical Review B, 2017, 95, .	3.2	31
12	First-principles study of high-conductance DNA sequencing with carbon nanotube electrodes. Physical Review B, 2012, 85, .	3.2	30
13	Prediction of large bias-dependent magnetoresistance in all-oxide magnetic tunnel junctions with a ferroelectric barrier. Physical Review B, 2011, 83, .	3.2	25
14	Evaluating the noise resilience of variational quantum algorithms. Physical Review A, 2021, 104, .	2.5	25
15	Stable anchoring chemistry for room temperature charge transport through graphite-molecule contacts. Science Advances, 2017, 3, e1602297.	10.3	23
16	Current-induced energy barrier suppression for electromigration from first principles. Physical Review B, 2011, 84, .	3.2	22
17	Predicting the conductance of strongly correlated molecules: the Kondo effect in perchlorotriphenylmethyl/Au junctions. Nanoscale, 2018, 10, 17738-17750.	5.6	22
18	Topological surface states scattering in antimony. Physical Review B, 2012, 86, .	3.2	21

#	Article	IF	Citations
19	Quantum conductance of a single magnetic atom: Anab initiostudy. Physical Review B, 2010, 82, .	3.2	19
20	Quantum state discrimination using noisy quantum neural networks. Physical Review Research, 2021, 3, .	3.6	19
21	Transmission through correlated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mtext>Cu</mml:mtext><mml:mi>n</mml:mi> Physical Review B, 2015, 92, .	3.2	15
22	Ab initiotransport across bismuth selenide surface barriers. Physical Review B, 2014, 90, .	3.2	14
23	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
24	Fundamental gap of molecular crystals via constrained density functional theory. Physical Review B, 2016, 93, .	3.2	13
25	The image charge effect and vibron-assisted processes in Coulomb blockade transport: a first principles approach. Nanoscale, 2015, 7, 19231-19240.	5.6	8
26	Electronic Transport as a Driver for Self-Interaction-Corrected Methods. Advances in Atomic, Molecular and Optical Physics, 2015, 64, 29-86.	2.3	7
27	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
28	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:msub><mml:mi mathvariant="normal">Î£</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> method for electron correlation effects at transition metal surfaces. Physical Review B, 2022, 105, .	3.2	7
29	Maximally localized dynamical quantum embedding for solving many-body correlated systems. Nature Computational Science, 2021, 1, 410-420.	8.0	6
30	Non-equilibrium Greenâ€™s Function Methods for Spin Transport and Dynamics. , 2020, , 957-983.		5
31	Spin-orbit induced equilibrium spin currents in materials. Physical Review B, 2022, 105, .	3.2	3
32	Non-equilibrium Greenâ€™s Function Methods for Spin Transport and Dynamics. , 2018, , 1-27.		2
33	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
34	Pressure-induced electronic transitions in samarium monochalcogenides. Physical Review B, 2022, 105, .	3.2	2
35	Enhanced thermopower in covalent graphiteâ€“molecule contacts. Physical Chemistry Chemical Physics, 2020, 22, 1466-1474.	2.8	1
36	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