Stefano Sanvito

List of Publications by Year
in descending order

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387 papers	23,892 citations	10984 71 h-index	8864 145 g-index
395 all docs	395 docs citations	395 times ranked	25029 citing authors

#	Article	IF	Citations
1	The high-throughput highway to computational materials design. Nature Materials, 2013, 12, 191-201.	27.5	1,475
2	Towards molecular spintronics. Nature Materials, 2005, 4, 335-339.	27.5	1,204
3	Molecular spintronics. Chemical Society Reviews, 2011, 40, 3336.	38.1	1,093
4	Liquid exfoliation of solvent-stabilized few-layer black phosphorus for applications beyond electronics. Nature Communications, 2015, 6, 8563.	12.8	921
5	AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. Computational Materials Science, 2012, 58, 227-235.	3.0	811
6	Solvent Exfoliation of Transition Metal Dichalcogenides: Dispersibility of Exfoliated Nanosheets Varies Only Weakly between Compounds. ACS Nano, 2012, 6, 3468-3480.	14.6	625
7	Spin and molecular electronics in atomically generated orbital landscapes. Physical Review B, 2006, 73, .	3.2	623
8	Hybrid Graphene and Graphitic Carbon Nitride Nanocomposite: Gap Opening, Electronâ€“Hole Puddle, Interfacial Charge Transfer, and Enhanced Visible Light Response. Journal of the American Chemical Society, 2012, 134, 4393-4397.	13.7	565
9	Revealing the role of organic cations in hybrid halide perovskite CH3NH3PbI3. Nature Communications, 2015, 6, 7026.	12.8	564
10	Possible doping strategies for MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>monolayers: Anab initiostudy. Physical Review B, 2013, 88, .	3.2	489
11	Ferromagnetism Driven by Intrinsic Point Defects inHfO2. Physical Review Letters, 2005, 94, 217205.	7.8	409
12	The rise of spinterface science. Nature Physics, 2010, 6, 562-564.	16.7	377
13	The role of anharmonic phonons in under-barrier spin relaxation of single molecule magnets. Nature Communications, 2017, 8, 14620.	12.8	319
14	Charge carrier mobility in hybrid halide perovskites. Scientific Reports, 2015, 5, 12746.	3.3	294
15	Basal-Plane Functionalization of Chemically Exfoliated Molybdenum Disulfide by Diazonium Salts. ACS Nano, 2015, 9, 6018-6030.	14.6	293
16	General Greenâ€™s-function formalism for transport calculations withspdHamiltonians and giant magnetoresistance in Co- and Ni-based magnetic multilayers. Physical Review B, 1999, 59, 11936-11948.	3.2	292
17	Self-Interaction Errors in Density-Functional Calculations of Electronic Transport. Physical Review Letters, 2005, 95, 146402.	7.8	292
18	First-Principles Prediction of a Room-Temperature Ferromagnetic Janus VSSe Monolayer with Piezoelectricity, Ferroelasticity, and Large Valley Polarization. Nano Letters, 2019, 19, 1366-1370.	9.1	292

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19	First-principles study of the origin and nature of ferromagnetism inGa1â^'xMnxAs. Physical Review B, 2001, 63, .	3.2	288
20	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
21	First-Principles Prediction of Metal-Free Magnetism and Intrinsic Half-Metallicity in Graphitic Carbon Nitride. Physical Review Letters, 2012, 108, 197207.	7.8	272
22	Origin of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-type and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type conductivity of MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>monolayers on a SiO<mml:math xmlns:mml="http://w	3.2	257
23	Ground state of half-metallic zinc-blende MnAs. Physical Review B, 2000, 62, 15553-15560.	3.2	227
24	Mixed Low-Dimensional Nanomaterial: 2D Ultranarrow MoS₂ Inorganic Nanoribbons Encapsulated in Quasi-1D Carbon Nanotubes. Journal of the American Chemical Society, 2010, 132, 13840-13847.	13.7	218
25	Accelerated discovery of new magnets in the Heusler alloy family. Science Advances, 2017, 3, e1602241.	10.3	197
26	Quantum Hall effect based on Weyl orbits in Cd3As2. Nature, 2019, 565, 331-336.	27.8	194
27	Electric Field Effects on Armchair MoS₂ Nanoribbons. ACS Nano, 2012, 6, 4823-4834.	14.6	187
28	Raman characterization of platinum diselenide thin films. 2D Materials, 2016, 3, 021004.	4.4	172
29	Fractional Quantum Conductance in Carbon Nanotubes. Physical Review Letters, 2000, 84, 1974-1977.	7.8	166
30	The 2020 magnetism roadmap. Journal Physics D: Applied Physics, 2020, 53, 453001.	2.8	162
31	Intra-molecular origin of the spin-phonon coupling in slow-relaxing molecular magnets. Chemical Science, 2017, 8, 6051-6059.	7.4	160
32	Impurity-ion pair induced high-temperature ferromagnetism in Co-doped ZnO. Physical Review B, 2008, 78, .	3.2	154
33	Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids. Physical Review B, 2007, 75, .	3.2	150
34	Magnetic semiconductors and half-metals. Journal Physics D: Applied Physics, 2004, 37, 988-993.	2.8	149
35	Zeeman splitting and dynamical mass generation in Dirac semimetal ZrTe5. Nature Communications, 2016, 7, 12516.	12.8	149
36	Electrostatic spin crossover effect in polar magnetic molecules. Nature Materials, 2009, 8, 813-817.	27.5	148

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37	A spin of their own. Nature Materials, 2009, 8, 693-695.	27.5	147
38	Electronic properties of bulk and thin film<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrRuO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:r Search for the metal-insulator transition. Physical Review B, 2008, 78, .	3.2	143
39	Spin-Valve Effect in NiFe/MoS₂/NiFe Junctions. Nano Letters, 2015, 15, 5261-5267.	9.1	135
40	Novel One-Dimensional Organometallic Half Metals: Vanadium-Cyclopentadienyl, Vanadium-Cyclopentadienyl-Benzene, and Vanadium-Anthracene Wires. Nano Letters, 2008, 8, 3640-3644.	9.1	131
41	Molecular-Spintronics: The Art of Driving Spin Through Molecules. Journal of Computational and Theoretical Nanoscience, 2006, 3, 624-642.	0.4	129
42	Predicting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mtext>d</mml:mtext><mml:mn>0</mml:mn></mml:msup></mml:mrow></mml:math Self-interaction correction scheme. Physical Review B, 2008, 78, .	3.2	124
43	Efficient Atomic Self-Interaction Correction Scheme for Nonequilibrium Quantum Transport. Physical Review Letters, 2007, 99, 056801.	7.8	123
44	Effects of self-interaction corrections on the transport properties of phenyl-based molecular junctions. Physical Review B, 2008, 77, .	3.2	121
45	Molecular-Spintronics: The Art of Driving Spin Through Molecules. Journal of Computational and Theoretical Nanoscience, 2006, 3, 624-642.	0.4	120
46	Evolution of Weyl orbit and quantum Hall effect in Dirac semimetal Cd3As2. Nature Communications, 2017, 8, 1272.	12.8	118
47	Different origins of the ferromagnetic order in (Ga,Mn)As and (Ga,Mn)N. Physical Review B, 2004, 70, .	3.2	114
48	Influence of Quantum Confinement on the Electronic and Magnetic Properties of (Ga,Mn)As Diluted Magnetic Semiconductor. Nano Letters, 2002, 2, 605-608.	9.1	101
49	Spintronics goes plastic. Nature Materials, 2007, 6, 803-804.	27.5	101
50	Molecular Kondo Chain. Nano Letters, 2012, 12, 3174-3179.	9.1	101
51	Giant Resistance Change across the Phase Transition in Spin-Crossover Molecules. Physical Review Letters, 2012, 108, 217201.	7.8	100
52	Predicting Single-Layer Technetium Dichalcogenides (TcX₂, X = S, Se) with Promising Applications in Photovoltaics and Photocatalysis. ACS Applied Materials & Interfaces, 2016, 8, 5385-5392.	8.0	100
53	Contact induced magnetism in carbon nanotubes. Journal of Physics Condensed Matter, 2004, 16, L155-L161.	1.8	95
54	On-site approximation for spinâ€“orbit coupling in linear combination of atomic orbitals density functional methods. Journal of Physics Condensed Matter, 2006, 18, 7999-8013.	1.8	95

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55	Assessment of density functional theory for iron(II) molecules across the spin-crossover transition. Journal of Chemical Physics, 2012, 137, 124303.	3.0	94
56	Materials informatics. Journal of Intelligent Manufacturing, 2019, 30, 2307-2326.	7.3	90
57	Ab Initio Calculations of Structural Evolution and Conductance of Benzene-1,4-dithiol on Gold Leads. ACS Nano, 2011, 5, 795-804.	14.6	89
58	Magnetic and electronic properties of D22-Mn3Ge (001) films. Applied Physics Letters, 2012, 101, .	3.3	88
59	Femtosecond Spin Current Pulses Generated by the Nonthermal Spin-Dependent Seebeck Effect and Interacting with Ferromagnets in Spin Valves. Physical Review Letters, 2017, 119, 017202.	7.8	86
60	Efficient spin injection and giant magnetoresistance in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">Fe</mml:mi><mml:mo>/</mml:mo><mml:mi mathvariant="normal">MoS</mml:mi><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:mi mathvariant="normal">Fe</mml:mi></mml:math>junctions. Physical Review B, 2014, 90, .	3.2	85
61	First-Principles Prediction of Spin-Polarized Multiple Dirac Rings in Manganese Fluoride. Physical Review Letters, 2017, 119, 016403.	7.8	84
62	Variational pseudo-self-interaction-corrected density functional approach to theab initiodescription of correlated solids and molecules. Physical Review B, 2011, 84, .	3.2	83
63	Density Functional Calculations for IIIâ€“V Diluted Ferromagnetic Semiconductors: A Review. Journal of Superconductivity and Novel Magnetism, 2002, 15, 85-104.	0.5	82
64	Site-specific order and magnetism in tetragonal Mn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>Ga thin films. Physical Review B, 2013, 87, .	3.2	81
65	Injecting and controlling spins in organic materials. Journal of Materials Chemistry, 2007, 17, 4455.	6.7	79
66	Molecular conduction: Do time-dependent simulations tell you more than the Landauer approach?. Journal of Chemical Physics, 2006, 124, 214708.	3.0	75
67	Effects induced by single and multiple dopants on the transport properties in zigzag-edged graphene nanoribbons. Physical Review B, 2009, 80, .	3.2	74
68	How do phonons relax molecular spins?. Science Advances, 2019, 5, eaax7163.	10.3	74
69	Functionalized Nanopore-Embedded Electrodes for Rapid DNA Sequencing. Journal of Physical Chemistry C, 2008, 112, 3456-3459.	3.1	73
70	Electric Field Control of Valence Tautomeric Interconversion in Cobalt Dioxolene. Physical Review Letters, 2011, 107, 047201.	7.8	73
71	Electron doping and magnetic moment formation in N- and C-doped MgO. Applied Physics Letters, 2009, 94, .	3.3	72
72	Spin-filtering efficiency of ferrimagnetic spinels CoFe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and NiFe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	3.2	71

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73	Polaronic distortion and vacancy-induced magnetism in MgO. Physical Review B, 2010, 81, .	3.2	70
74	Influence of the local As antisite distribution on ferromagnetism in (Ga,â€ŠMn)As. Applied Physics Letters, 2001, 78, 3493-3495.	3.3	69
75	AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. Journal of Chemical Information and Modeling, 2018, 58, 2477-2490.	5.4	69
76	Gate-tunable quantum oscillations in ambipolar Cd3As2 thin films. NPG Asia Materials, 2015, 7, e221-e221.	7.9	68
77	Ultrahigh conductivity in Weyl semimetal NbAs nanobelts. Nature Materials, 2019, 18, 482-488.	27.5	68
78	Spin transport properties of 3d transition metal(ii) phthalocyanines in contact with single-walled carbon nanotube electrodes. Physical Chemistry Chemical Physics, 2010, 12, 10805.	2.8	66
79	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advancedab initiomethods. Physical Review B, 2011, 84, .	3.2	66
80	Filtering spins with molecules. Nature Materials, 2011, 10, 484-485.	27.5	63
81	Switching a Single Spin on Metal Surfaces by a STM Tip:AbÂInitioStudies. Physical Review Letters, 2009, 103, 057202.	7.8	60
82	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:m Physical Review B, 2009, 80, .	3.2	60
83	First-Principles Investigation of Spinâ€“Phonon Coupling in Vanadium-Based Molecular Spin Quantum Bits. Inorganic Chemistry, 2019, 58, 10260-10268.	4.0	59
84	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>curv of Fe/MgO/Fe(100) tunnel junctions. Physical Review B, 2009, 79, .	3.2	57
85	Conductance Oscillations in Zigzag Platinum Chains. Physical Review Letters, 2005, 95, 256804.	7.8	56
86	Polarizability of molecular chains: A self-interaction correction approach. Physical Review B, 2008, 77, .	3.2	56
87	Spin filter effect of manganese phthalocyanine contacted with single-walled carbon nanotube electrodes. Journal of Chemical Physics, 2010, 132, 054703.	3.0	56
88	Dynamic spin filtering at the Co/Alq3 interface mediated by weakly coupled second layer molecules. Nature Communications, 2016, 7, 12668.	12.8	55
89	Constrained-DFT method for accurate energy-level alignment of metal/molecule interfaces. Physical Review B, 2013, 88, .	3.2	54
90	Topological Tuning in Three-Dimensional Dirac Semimetals. Physical Review Letters, 2014, 113, 256403.	7.8	53

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91	Spin-Polarized Tunneling through Chemical Vapor Deposited Multilayer Molybdenum Disulfide. ACS Nano, 2017, 11, 6389-6395.	14.6	53
92	Observation of quasi-two-dimensional Dirac fermions in ZrTe5. NPG Asia Materials, 2016, 8, e325-e325.	7.9	51
93	Prediction of room-temperature ferromagnetism and large perpendicular magnetic anisotropy in a planar hypercoordinate FeB₃monolayer. Nanoscale Horizons, 2021, 6, 43-48.	8.0	50
94	AsymmetricIâˆ'Vcharacteristics and magnetoresistance in magnetic point contacts. Physical Review B, 2004, 70, .	3.2	49
95	Improving stability of organometallic-halide perovskite solar cells using exfoliation two-dimensional molybdenum chalcogenides. Npj 2D Materials and Applications, 2020, 4, .	7.9	49
96	Multiple spinâ€“phonon relaxation pathways in a Kramer single-ion magnet. Journal of Chemical Physics, 2020, 153, 174113.	3.0	49
97	Prediction of the two-dimensional Janus ferrovalley material LaBrI. Physical Review B, 2021, 104, .	3.2	49
98	Predicting the Curie temperature of ferromagnets using machine learning. Physical Review Materials, 2019, 3, .	2.4	49
99	Inducing Strong Superconductivity in WTe₂ by a Proximity Effect. ACS Nano, 2018, 12, 7185-7196.	14.6	48
100	An efficient nonequilibrium Greenâ€™s function formalism combined with density functional theory approach for calculating electron transport properties of molecular devices with quasi-one-dimensional electrodes. Journal of Chemical Physics, 2007, 127, 194710.	3.0	47
101	Electronic Properties and Chemical Reactivity of TiS₂ Nanoflakes. Journal of Physical Chemistry C, 2015, 119, 15707-15715.	3.1	47
102	Spin scattering and spin-polarized hybrid interface states at a metal-organic interface. Physical Review B, 2011, 84, .	3.2	46
103	Nucleobase adsorbed at graphene devices: Enhance bio-sensorics. Applied Physics Letters, 2012, 100, 063101.	3.3	45
104	Exploring new approaches towards the formability of mixed-ion perovskites by DFT and machine learning. Physical Chemistry Chemical Physics, 2019, 21, 1078-1088.	2.8	45
105	Ab InitioTransport Theory for Digital Ferromagnetic Heterostructures. Physical Review Letters, 2001, 87, 267202.	7.8	44
106	The Limit of Spin Lifetime in Solid-State Electronic Spins. Journal of Physical Chemistry Letters, 2020, 11, 6273-6278.	4.6	44
107	Ab initiostudy of the magnetostructural properties of MnAs. Physical Review B, 2006, 74, .	3.2	43
108	Unusual Stacking Variations in Liquid-Phase Exfoliated Transition Metal Dichalcogenides. ACS Nano, 2014, 8, 3690-3699.	14.6	43

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109	Dimensionality-driven phonon softening and incipient charge density wave instability in TiS ₂. Europhysics Letters, 2016, 115, 47001.	2.0	43
110	Unveiling phonons in a molecular qubit with four-dimensional inelastic neutron scattering and density functional theory. Nature Communications, 2020, 11, 1751.	12.8	43
111	Single-channel conductance ofH2molecules attached to platinum or palladium electrodes. Physical Review B, 2005, 72, .	3.2	42
112	Observation of van der Waals Driven Self-Assembly of MoSI Nanowires into a Low-Symmetry Structure Using Aberration-Corrected Electron Microscopy. Advanced Materials, 2007, 19, 543-547.	21.0	42
113	Finite-bias electronic transport of molecules in a water solution. Physical Review B, 2010, 81, .	3.2	42
114	Exceptionally strong magnetism in the 4<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>d</mml:mi></mml:mrow></mml:math>perovskites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>R</mml:mi></mml:mrow></mml:math>TcO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:m	3.2	42
115	Machine Learning Accelerated Recovery of the Cubic Structure in Mixed-Cation Perovskite Thin Films. Chemistry of Materials, 2020, 32, 2998-3006.	6.7	42
116	Coexistance of Giant Tunneling Electroresistance and Magnetoresistance in an All-Oxide Composite Magnetic Tunnel Junction. Physical Review Letters, 2012, 109, 226803.	7.8	41
117	Electronic and magnetic properties of the interface between metal-quinoline molecules and cobalt. Physical Review B, 2014, 89, .	3.2	41
118	Investigation of the Conducting Properties of a Photoswitching Dithienylethene Molecule. ACS Nano, 2010, 4, 2635-2642.	14.6	40
119	Geâ€Based Spinâ€Photodiodes for Roomâ€Temperature Integrated Detection of Photon Helicity. Advanced Materials, 2012, 24, 3037-3041.	21.0	40
120	Stretching of BDT-gold molecular junctions: thiol or thiolate termination?. Nanoscale, 2014, 6, 14495-14507.	5.6	40
121	Exploring the cation dynamics in lead-bromide hybrid perovskites. Physical Review B, 2016, 93, .	3.2	40
122	Efficientab initiomethod for inelastic transport in nanoscale devices: Analysis of inelastic electron tunneling spectroscopy. Physical Review B, 2008, 78, .	3.2	39
123	Self-interaction effects in (Ga,Mn)As and (Ga,Mn)N. Chemical Physics, 2005, 309, 59-65.	1.9	38
124	Atomistic simulations of highly conductive molecular transport junctions under realistic conditions. Nanoscale, 2013, 5, 3654.	5.6	38
125	Magnetism of CoO polymorphs: Density functional theory and Monte Carlo simulations. Physical Review B, 2008, 78, .	3.2	37
126	Controlling the Spin Texture of Topological Insulators by Rational Design of Organic Molecules. Nano Letters, 2015, 15, 6022-6029.	9.1	37

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127	Resistive switching mechanism of GeTeâ€“Sb₂Te₃ interfacial phase change memory and topological properties of embedded two-dimensional states. Nanoscale, 2017, 9, 9386-9395.	5.6	36
128	Electronic Transport Properties of 1,1â€²-Ferrocene Dicarboxylic Acid Linked to Al(111) Electrodes. ACS Nano, 2009, 3, 4137-4143.	14.6	35
129	Memoirs of a spin. Nature Nanotechnology, 2007, 2, 204-206.	31.5	34
130	The spin filter effect of iron-cyclopentadienyl multidecker clusters: the role of the electrode band structure and the coupling strength. Nanotechnology, 2009, 20, 385401.	2.6	34
131	Designing a fully compensated half-metallic ferrimagnet. Physical Review B, 2016, 93, .	3.2	34
132	Structural Origins of Conductance Fluctuations in Goldâ€“Thiolate Molecular Transport Junctions. Journal of Physical Chemistry Letters, 2013, 4, 887-891.	4.6	33
133	A unified picture of the covalent bond within quantum-accurate force fields: From organic molecules to metallic complexesâ€™ reactivity. Science Advances, 2019, 5, eaaw2210.	10.3	33
134	Exploring the limits of the self-consistent Born approximation for inelastic electronic transport. Physical Review B, 2009, 79, .	3.2	32
135	Half-Metallic Sandwich Molecular Wires with Negative Differential Resistance and Sign-Reversible High Spin-Filter Efficiency. Journal of Physical Chemistry C, 2010, 114, 21893-21899.	3.1	32
136	Tuning the Magneto-Transport Properties of Nickelâ^'Cyclopentadienyl Multidecker Clusters by Moleculeâ^'Electrode Coupling Manipulation. ACS Nano, 2010, 4, 2274-2282.	14.6	32
137	Replacement and Original Magnet Engineering Options (ROMEOs): A European Seventh Framework Project to Develop Advanced Permanent Magnets Without, or with Reduced Use of, Critical Raw Materials. Jom, 2015, 67, 1306-1317.	1.9	31
138	First-principles spin-transfer torque in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CuMnAs</mml:mi><mml:mo>|</mml:mo><mml:mi>GaP</mml:mi></mml:mrow></mml:math> junctions. Physical Review B, 2017, 95, .	3.2	31
139	First-principles study of high-conductance DNA sequencing with carbon nanotube electrodes. Physical Review B, 2012, 85, .	3.2	30
140	MgN: A possible material for spintronic applications. Physical Review B, 2009, 80, .	3.2	29
141	Spin transport in higher<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-acene molecules. Physical Review B, 2011, 84, .	3.2	29
142	Electronâ€“Phonon Coupling and Polaron Mobility in Hybrid Perovskites from First Principles. Journal of Physical Chemistry C, 2018, 122, 1361-1366.	3.1	29
143	Machine learning density functional theory for the Hubbard model. Physical Review B, 2019, 99, .	3.2	29
144	Electric-controlled half-metallicity in magnetic van der Waals heterobilayer. Journal of Materials Chemistry C, 2020, 8, 7034-7040.	5.5	29

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145	Ab initiostudy of electron transport in dry poly(G)-poly(C)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>A</mml:mi></mml:math>-DNA strands. Physical Review B, 2010, 82, .	3.2	28
146	Effects of edge chemistry doping on graphene nanoribbon mobility. Surface Science, 2011, 605, 1643-1648.	1.9	28
147	Learn-and-Match Molecular Cations for Perovskites. Journal of Physical Chemistry A, 2019, 123, 7323-7334.	2.5	28
148	Low-bias conductance of single benzene molecules contacted by direct Auâ€“C and Ptâ€“C bonds. Nanotechnology, 2010, 21, 495202.	2.6	27
149	Contact-induced spin polarization in carbon nanotubes. Physical Review B, 2004, 69, .	3.2	26
150	First-principles calculation on the zero-bias conductance of a gold/1,4-diaminobenzene/gold molecular junction. Nanotechnology, 2007, 18, 345203.	2.6	26
151	Magnetic properties of ZrO2-diluted magnetic semiconductors. Journal of Magnetism and Magnetic Materials, 2007, 316, e188-e190.	2.3	26
152	Diffusion Monte Carlo Perspective on the Spin-State Energetics of [Fe(NCH)₆]²⁺. Journal of Chemical Theory and Computation, 2016, 12, 4233-4241.	5.3	26
153	Prediction of large bias-dependent magnetoresistance in all-oxide magnetic tunnel junctions with a ferroelectric barrier. Physical Review B, 2011, 83, .	3.2	25
154	Efficient conducting channels formed by the Ï€-Ï€ stacking in single [2,2]paracyclophane molecules. Journal of Chemical Physics, 2012, 136, 104701.	3.0	25
155	Ab initiotheory for current-induced molecular switching: Melamine on Cu(001). Physical Review B, 2013, 87, .	3.2	25
156	Lattice Distortion Effects on the Magnetostructural Phase Transition of MnAs. Physical Review Letters, 2005, 95, 077203.	7.8	24
157	Conceptual molecular quantum phase transistor based on first-principles quantum transport calculations. Physical Review B, 2008, 78, .	3.2	24
158	Newtonian origin of the spin motive force in ferromagnetic atomic wires. Physical Review B, 2008, 77, .	3.2	24
159	Effects of structural relaxation on calculations of the interface and transport properties of Fe/MgO(001) tunnel junctions. Physical Review B, 2009, 79, .	3.2	24
160	Simulating STM transport in alkanes from first principles. Physical Review B, 2009, 79, .	3.2	24
161	Vertical Single-Crystalline Organic Nanowires on Graphene: Solution-Phase Epitaxy and Optical Microcavities. Nano Letters, 2016, 16, 4754-4762.	9.1	24
162	Multiscale modeling of current-induced switching in magnetic tunnel junctions using ab initio spin-transfer torques. Physical Review B, 2017, 96, .	3.2	24

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