

Stefano Sanvito

List of Publications by Year in descending order

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387
papers

23,892
citations

10956

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8835

145
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395
all docs

395
docs citations

395
times ranked

25029
citing authors

#	ARTICLE	IF	CITATIONS
1	The high-throughput highway to computational materials design. <i>Nature Materials</i> , 2013, 12, 191-201.	13.3	1,475
2	Towards molecular spintronics. <i>Nature Materials</i> , 2005, 4, 335-339.	13.3	1,204
3	Molecular spintronics. <i>Chemical Society Reviews</i> , 2011, 40, 3336.	18.7	1,093
4	Liquid exfoliation of solvent-stabilized few-layer black phosphorus for applications beyond electronics. <i>Nature Communications</i> , 2015, 6, 8563.	5.8	921
5	AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. <i>Computational Materials Science</i> , 2012, 58, 227-235.	1.4	811
6	Solvent Exfoliation of Transition Metal Dichalcogenides: Dispersibility of Exfoliated Nanosheets Varies Only Weakly between Compounds. <i>ACS Nano</i> , 2012, 6, 3468-3480.	7.3	625
7	Spin and molecular electronics in atomically generated orbital landscapes. <i>Physical Review B</i> , 2006, 73, .	1.1	623
8	Hybrid Graphene and Graphitic Carbon Nitride Nanocomposite: Gap Opening, Electronâ€“Hole Puddle, Interfacial Charge Transfer, and Enhanced Visible Light Response. <i>Journal of the American Chemical Society</i> , 2012, 134, 4393-4397.	6.6	565
9	Revealing the role of organic cations in hybrid halide perovskite CH ₃ NH ₃ PbI ₃ . <i>Nature Communications</i> , 2015, 6, 7026.	5.8	564
10	Possible doping strategies for MoS ₂ monolayers: An ab initio study. <i>Physical Review B</i> , 2013, 88, .	1.1	489
11	Ferromagnetism Driven by Intrinsic Point Defects in HfO ₂ . <i>Physical Review Letters</i> , 2005, 94, 217205.	2.9	409
12	The rise of spinterface science. <i>Nature Physics</i> , 2010, 6, 562-564.	6.5	377
13	The role of anharmonic phonons in under-barrier spin relaxation of single molecule magnets. <i>Nature Communications</i> , 2017, 8, 14620.	5.8	319
14	Charge carrier mobility in hybrid halide perovskites. <i>Scientific Reports</i> , 2015, 5, 12746.	1.6	294
15	Basal-Plane Functionalization of Chemically Exfoliated Molybdenum Disulfide by Diazonium Salts. <i>ACS Nano</i> , 2015, 9, 6018-6030.	7.3	293
16	General Greenâ€™s-function formalism for transport calculations with spd Hamiltonians and giant magnetoresistance in Co- and Ni-based magnetic multilayers. <i>Physical Review B</i> , 1999, 59, 11936-11948.	1.1	292
17	Self-Interaction Errors in Density-Functional Calculations of Electronic Transport. <i>Physical Review Letters</i> , 2005, 95, 146402.	2.9	292
18	First-Principles Prediction of a Room-Temperature Ferromagnetic Janus VSSe Monolayer with Piezoelectricity, Ferroelasticity, and Large Valley Polarization. <i>Nano Letters</i> , 2019, 19, 1366-1370.	4.5	292

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19	First-principles study of the origin and nature of ferromagnetism in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$. Physical Review B, 2001, 63, .	1.1	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, .	1.1	279
21	First-Principles Prediction of Metal-Free Magnetism and Intrinsic Half-Metallicity in Graphitic Carbon Nitride. Physical Review Letters, 2012, 108, 197207	2.9	272
22	Origin of the n -type and p -type conductivity of MoS_2 monolayers on a SiO_2	1.1	257
23	Ground state of half-metallic zinc-blende MnAs . Physical Review B, 2000, 62, 15553-15560.	1.1	227
24	Mixed Low-Dimensional Nanomaterial: 2D Ultranarrow MoS_2 Inorganic Nanoribbons Encapsulated in Quasi-1D Carbon Nanotubes. Journal of the American Chemical Society, 2010, 132, 13840-13847.	6.6	218
25	Accelerated discovery of new magnets in the Heusler alloy family. Science Advances, 2017, 3, e1602241.	4.7	197
26	Quantum Hall effect based on Weyl orbits in Cd_3As_2 . Nature, 2019, 565, 331-336.	13.7	194
27	Electric Field Effects on Armchair MoS_2 Nanoribbons. ACS Nano, 2012, 6, 4823-4834.	7.3	187
28	Raman characterization of platinum diselenide thin films. 2D Materials, 2016, 3, 021004.	2.0	172
29	Fractional Quantum Conductance in Carbon Nanotubes. Physical Review Letters, 2000, 84, 1974-1977.	2.9	166
30	The 2020 magnetism roadmap. Journal Physics D: Applied Physics, 2020, 53, 453001.	1.3	162
31	Intra-molecular origin of the spin-phonon coupling in slow-relaxing molecular magnets. Chemical Science, 2017, 8, 6051-6059.	3.7	160
32	Impurity-ion pair induced high-temperature ferromagnetism in Co-doped ZnO . Physical Review B, 2008, 78, .	1.1	154
33	Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids. Physical Review B, 2007, 75, .	1.1	150
34	Magnetic semiconductors and half-metals. Journal Physics D: Applied Physics, 2004, 37, 988-993.	1.3	149
35	Zeeman splitting and dynamical mass generation in Dirac semimetal ZrTe_5 . Nature Communications, 2016, 7, 12516.	5.8	149
36	Electrostatic spin crossover effect in polar magnetic molecules. Nature Materials, 2009, 8, 813-817.	13.3	148

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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.	1.2	94
56	Materials informatics. Journal of Intelligent Manufacturing, 2019, 30, 2307-2326.	4.4	90
57	Ab Initio Calculations of Structural Evolution and Conductance of Benzene-1,4-dithiol on Gold Leads. ACS Nano, 2011, 5, 795-804.	7.3	89
58	Magnetic and electronic properties of D_{2d} -Mn ₃ Ge (001) films. Applied Physics Letters, 2012, 101, .	1.5	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.	2.9	86
60	Efficient spin injection and giant magnetoresistance in MoS_2 and Fe/MoS_2 junctions. Physical Review B, 2014, 90, .	1.1	85
61	First-Principles Prediction of Spin-Polarized Multiple Dirac Rings in Manganese Fluoride. Physical Review Letters, 2017, 119, 016403.	2.9	84
62	Variational pseudo-self-interaction-corrected density functional approach to the description of correlated solids and molecules. Physical Review B, 2011, 84, .	1.1	83
63	Density Functional Calculations for 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_3Ga thin films. Physical Review B, 2013, 87, .	1.1	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.	1.2	75
67	Effects induced by single and multiple dopants on the transport properties in zigzag-edged graphene nanoribbons. Physical Review B, 2009, 80, .	1.1	74
68	How do phonons relax molecular spins?. Science Advances, 2019, 5, eaax7163.	4.7	74
69	Functionalized Nanopore-Embedded Electrodes for Rapid DNA Sequencing. Journal of Physical Chemistry C, 2008, 112, 3456-3459.	1.5	73
70	Electric Field Control of Valence Tautomeric Interconversion in Cobalt Dioxolene. Physical Review Letters, 2011, 107, 047201.	2.9	73
71	Electron doping and magnetic moment formation in N- and C-doped MgO. Applied Physics Letters, 2009, 94, .	1.5	72
72	Spin-filtering efficiency of ferrimagnetic spinels $CoFe_2O_4$ and $NiFe_2O_4$. Physical Review Letters, 2011, 107, 047201.	1.1	71

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91	Spin-Polarized Tunneling through Chemical Vapor Deposited Multilayer Molybdenum Disulfide. ACS Nano, 2017, 11, 6389-6395.	7.3	53
92	Observation of quasi-two-dimensional Dirac fermions in ZrTe5. NPC Asia Materials, 2016, 8, e325-e325.	3.8	51
93	Prediction of room-temperature ferromagnetism and large perpendicular magnetic anisotropy in a planar hypercoordinate FeB ₃ monolayer. Nanoscale Horizons, 2021, 6, 43-48.	4.1	50
94	Asymmetric characteristics and magnetoresistance in magnetic point contacts. Physical Review B, 2004, 70, .	1.1	49
95	Improving stability of organometallic-halide perovskite solar cells using exfoliation two-dimensional molybdenum chalcogenides. Npj 2D Materials and Applications, 2020, 4, .	3.9	49
96	Multiple spin-phonon relaxation pathways in a Kramer single-ion magnet. Journal of Chemical Physics, 2020, 153, 174113.	1.2	49
97	Prediction of the two-dimensional Janus ferrovalley material LaBr. Physical Review B, 2021, 104, .	1.1	49
98	Predicting the Curie temperature of ferromagnets using machine learning. Physical Review Materials, 2019, 3, .	0.9	49
99	Inducing Strong Superconductivity in WTe ₂ by a Proximity Effect. ACS Nano, 2018, 12, 7185-7196.	7.3	48
100	An efficient nonequilibrium Green'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.	1.2	47
101	Electronic Properties and Chemical Reactivity of TiS ₂ Nanoflakes. Journal of Physical Chemistry C, 2015, 119, 15707-15715.	1.5	47
102	Spin scattering and spin-polarized hybrid interface states at a metal-organic interface. Physical Review B, 2011, 84, .	1.1	46
103	Nucleobase adsorbed at graphene devices: Enhance bio-sensorics. Applied Physics Letters, 2012, 100, 063101.	1.5	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.	1.3	45
105	Ab Initio Transport Theory for Digital Ferromagnetic Heterostructures. Physical Review Letters, 2001, 87, 267202.	2.9	44
106	The Limit of Spin Lifetime in Solid-State Electronic Spins. Journal of Physical Chemistry Letters, 2020, 11, 6273-6278.	2.1	44
107	Ab initio study of the magnetostructural properties of MnAs. Physical Review B, 2006, 74, .	1.1	43
108	Unusual Stacking Variations in Liquid-Phase Exfoliated Transition Metal Dichalcogenides. ACS Nano, 2014, 8, 3690-3699.	7.3	43

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109	Dimensionality-driven phonon softening and incipient charge density wave instability in TiS $\langle \text{sub} \rangle 2 \langle \text{/sub} \rangle$. <i>Europysics Letters</i> , 2016, 115, 47001.	0.7	43
110	Unveiling phonons in a molecular qubit with four-dimensional inelastic neutron scattering and density functional theory. <i>Nature Communications</i> , 2020, 11, 1751.	5.8	43
111	Single-channel conductance of H ₂ molecules attached to platinum or palladium electrodes. <i>Physical Review B</i> , 2005, 72, .	1.1	42
112	Observation of van der Waals Driven Self-Assembly of MoSI Nanowires into a Low-Symmetry Structure Using Aberration-Corrected Electron Microscopy. <i>Advanced Materials</i> , 2007, 19, 543-547.	11.1	42
113	Finite-bias electronic transport of molecules in a water solution. <i>Physical Review B</i> , 2010, 81, .	1.1	42
114	Exceptionally strong magnetism in the 4 $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{display="inline"} \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{d} \langle \text{/mml:mi} \rangle \langle \text{/mml:mrow} \rangle \langle \text{/mml:math} \rangle$ perovskites $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{display="inline"} \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{R} \langle \text{/mml:mi} \rangle \langle \text{/mml:mrow} \rangle \langle \text{/mml:math} \rangle$ TcO $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{display="inline"} \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:m}$	1.1	42
115	Machine Learning Accelerated Recovery of the Cubic Structure in Mixed-Cation Perovskite Thin Films. <i>Chemistry of Materials</i> , 2020, 32, 2998-3006.	3.2	42
116	Coexistence of Giant Tunneling Electroresistance and Magnetoresistance in an All-Oxide Composite Magnetic Tunnel Junction. <i>Physical Review Letters</i> , 2012, 109, 226803.	2.9	41
117	Electronic and magnetic properties of the interface between metal-quinoline molecules and cobalt. <i>Physical Review B</i> , 2014, 89, .	1.1	41
118	Investigation of the Conducting Properties of a Photoswitching Dithienylethene Molecule. <i>ACS Nano</i> , 2010, 4, 2635-2642.	7.3	40
119	Geâ€Based Spinâ€Photodiodes for Roomâ€Temperature Integrated Detection of Photon Helicity. <i>Advanced Materials</i> , 2012, 24, 3037-3041.	11.1	40
120	Stretching of BDT-gold molecular junctions: thiol or thiolate termination?. <i>Nanoscale</i> , 2014, 6, 14495-14507.	2.8	40
121	Exploring the cation dynamics in lead-bromide hybrid perovskites. <i>Physical Review B</i> , 2016, 93, .	1.1	40
122	Efficient <i>ab initio</i> method for inelastic transport in nanoscale devices: Analysis of inelastic electron tunneling spectroscopy. <i>Physical Review B</i> , 2008, 78, .	1.1	39
123	Self-interaction effects in (Ga,Mn)As and (Ga,Mn)N. <i>Chemical Physics</i> , 2005, 309, 59-65.	0.9	38
124	Atomistic simulations of highly conductive molecular transport junctions under realistic conditions. <i>Nanoscale</i> , 2013, 5, 3654.	2.8	38
125	Magnetism of CoO polymorphs: Density functional theory and Monte Carlo simulations. <i>Physical Review B</i> , 2008, 78, .	1.1	37
126	Controlling the Spin Texture of Topological Insulators by Rational Design of Organic Molecules. <i>Nano Letters</i> , 2015, 15, 6022-6029.	4.5	37

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127	Resistive switching mechanism of GeTe ₂ Te ₃ interfacial phase change memory and topological properties of embedded two-dimensional states. <i>Nanoscale</i> , 2017, 9, 9386-9395.	2.8	36
128	Electronic Transport Properties of 1,1'-Ferrocene Dicarboxylic Acid Linked to Al(111) Electrodes. <i>ACS Nano</i> , 2009, 3, 4137-4143.	7.3	35
129	Memoirs of a spin. <i>Nature Nanotechnology</i> , 2007, 2, 204-206.	15.6	34
130	The spin filter effect of iron-cyclopentadienyl multidecker clusters: the role of the electrode band structure and the coupling strength. <i>Nanotechnology</i> , 2009, 20, 385401.	1.3	34
131	Designing a fully compensated half-metallic ferrimagnet. <i>Physical Review B</i> , 2016, 93, .	1.1	34
132	Structural Origins of Conductance Fluctuations in Gold-Thiolate Molecular Transport Junctions. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 887-891.	2.1	33
133	A unified picture of the covalent bond within quantum-accurate force fields: From organic molecules to metallic complexes' reactivity. <i>Science Advances</i> , 2019, 5, eaaw2210.	4.7	33
134	Exploring the limits of the self-consistent Born approximation for inelastic electronic transport. <i>Physical Review B</i> , 2009, 79, .	1.1	32
135	Half-Metallic Sandwich Molecular Wires with Negative Differential Resistance and Sign-Reversible High Spin-Filter Efficiency. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21893-21899.	1.5	32
136	Tuning the Magneto-Transport Properties of Nickel-Cyclopentadienyl Multidecker Clusters by Molecule-Electrode Coupling Manipulation. <i>ACS Nano</i> , 2010, 4, 2274-2282.	7.3	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. <i>Jom</i> , 2015, 67, 1306-1317.	0.9	31
138	First-principles spin-transfer torque in $\text{CuMnAs} \text{GaP}$ junctions. <i>Physical Review B</i> , 2017, 95, .		
139	First-principles study of high-conductance DNA sequencing with carbon nanotube electrodes. <i>Physical Review B</i> , 2012, 85, .	1.1	30
140	MgN: A possible material for spintronic applications. <i>Physical Review B</i> , 2009, 80, .	1.1	29
141	Spin transport in higher n -acene molecules. <i>Physical Review B</i> , 2011, 84, .	1.1	29
142	Electron-Phonon Coupling and Polaron Mobility in Hybrid Perovskites from First Principles. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1361-1366.	1.5	29
143	Machine learning density functional theory for the Hubbard model. <i>Physical Review B</i> , 2019, 99, .	1.1	29
144	Electric-controlled half-metallicity in magnetic van der Waals heterobilayer. <i>Journal of Materials Chemistry C</i> , 2020, 8, 7034-7040.	2.7	29

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145	<i>Ab initio</i> study of electron transport in dry poly(G)-poly(C) DNA strands. Physical Review B, 2010, 82, .	1.1	28
146	Effects of edge chemistry doping on graphene nanoribbon mobility. Surface Science, 2011, 605, 1643-1648.	0.8	28
147	Learn-and-Match Molecular Cations for Perovskites. Journal of Physical Chemistry A, 2019, 123, 7323-7334.	1.1	28
148	Low-bias conductance of single benzene molecules contacted by direct Au-C and Pt-C bonds. Nanotechnology, 2010, 21, 495202.	1.3	27
149	Contact-induced spin polarization in carbon nanotubes. Physical Review B, 2004, 69, .	1.1	26
150	First-principles calculation on the zero-bias conductance of a gold/1,4-diaminobenzene/gold molecular junction. Nanotechnology, 2007, 18, 345203.	1.3	26
151	Magnetic properties of ZrO ₂ -diluted magnetic semiconductors. Journal of Magnetism and Magnetic Materials, 2007, 316, e188-e190.	1.0	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.	2.3	26
153	Prediction of large bias-dependent magnetoresistance in all-oxide magnetic tunnel junctions with a ferroelectric barrier. Physical Review B, 2011, 83, .	1.1	25
154	Efficient conducting channels formed by the π - π stacking in single [2,2]paracyclophane molecules. Journal of Chemical Physics, 2012, 136, 104701.	1.2	25
155	<i>Ab initio</i> theory for current-induced molecular switching: Melamine on Cu(001). Physical Review B, 2013, 87, .	1.1	25
156	Lattice Distortion Effects on the Magnetostructural Phase Transition of MnAs. Physical Review Letters, 2005, 95, 077203.	2.9	24
157	Conceptual molecular quantum phase transistor based on first-principles quantum transport calculations. Physical Review B, 2008, 78, .	1.1	24
158	Newtonian origin of the spin motive force in ferromagnetic atomic wires. Physical Review B, 2008, 77, .	1.1	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, .	1.1	24
160	Simulating STM transport in alkanes from first principles. Physical Review B, 2009, 79, .	1.1	24
161	Vertical Single-Crystalline Organic Nanowires on Graphene: Solution-Phase Epitaxy and Optical Microcavities. Nano Letters, 2016, 16, 4754-4762.	4.5	24
162	Multiscale modeling of current-induced switching in magnetic tunnel junctions using <i>ab initio</i> spin-transfer torques. Physical Review B, 2017, 96, .	1.1	24

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163	Electric field modulation of magnetism in ferrimagnetic Heusler heterostructures. <i>Physical Review B</i> , 2020, 101, .	1.1	24
164	From zigzag to armchair: the energetic stability, electronic and magnetic properties of chiral graphene nanoribbons with hydrogen-terminated edges. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 425301.	0.7	23
165	Spin-flip inelastic electron tunneling spectroscopy in atomic chains. <i>Physical Review B</i> , 2011, 84, .	1.1	23
166	Ferroelectric control of electron half-metallicity in A -type antiferromagnets and its application to nonvolatile memory devices. <i>Physical Review B</i> , 2020, 102, .	1.1	23
167	The magnetism of carbon. <i>Physics World</i> , 2004, 17, 33-37.	0.0	22
168	Current-driven magnetic rearrangements in spin-polarized point contacts. <i>Physical Review B</i> , 2005, 72, .	1.1	22
169	Search for magnetoresistance in excess of 1000% in Ni point contacts: Density functional calculations. <i>Physical Review B</i> , 2007, 76, .	1.1	22
170	Perturbative approach to the Kondo effect in magnetic atoms on nonmagnetic substrates. <i>Physical Review B</i> , 2011, 84, .	1.1	22
171	Current-induced energy barrier suppression for electromigration from first principles. <i>Physical Review B</i> , 2011, 84, .	1.1	22
172	Many-body quasiparticle spectrum of Co-doped ZnO: A G W perspective. <i>Physical Review B</i> , 2013, 87, .	1.1	22
173	Role of spin-orbit interaction in the ultrafast demagnetization of small iron clusters. <i>Physical Review B</i> , 2016, 94, .	1.1	22
174	Strain-induced Weyl and Dirac states and direct-indirect gap transitions in group-V materials. <i>2D Materials</i> , 2017, 4, 045018.	2.0	22
175	Edge superconductivity in multilayer WTe ₂ Josephson junction. <i>National Science Review</i> , 2020, 7, 1468-1475.	4.6	22
176	Importance of structural deformation features in the prediction of hybrid perovskite bandgaps. <i>Computational Materials Science</i> , 2020, 184, 109858.	1.4	22
177	Surfing Multiple Conformation-Property Landscapes via Machine Learning: Designing Single-Ion Magnetic Anisotropy. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5802-5806.	1.5	22
178	Suppression of Giant Magnetoresistance by a Superconducting Contact. <i>Physical Review Letters</i> , 1999, 82, 4938-4941.	2.9	21
179	Ferromagnetism and metallic state in digital (Ga,Mn)As heterostructures. <i>Physical Review B</i> , 2003, 68, .	1.1	21
180	V curvature of Fe/MgO (001) single- and double-barrier tunnel junctions. <i>Physical Review B</i> , 2008, 78, .	1.1	21

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181	Topological surface states scattering in antimony. <i>Physical Review B</i> , 2012, 86, .	1.1	21
182	Electronic transport through EuO spin-filter tunnel junctions. <i>Physical Review B</i> , 2012, 86, .	1.1	21
183	Spin-dependent electronic structure of the Co/Al(OP) ₃ interface. <i>New Journal of Physics</i> , 2013, 15, 113054.	1.2	21
184	An in situ and ex situ TEM study into the oxidation of titanium (IV) sulphide. <i>Npj 2D Materials and Applications</i> , 2017, 1, .	3.9	21
185	Interface and transport properties of Fe/V/MgO/Fe and Fe/V/Fe/MgO/Fe magnetic tunneling junctions. <i>Physical Review B</i> , 2009, 79, .	1.1	20
186	Spin-polarized transport through single-molecule magnet Mn ₆ complexes. <i>Nanoscale</i> , 2013, 5, 4751.	2.8	20
187	Origin of the p-Type Character of AuCl ₃ Functionalized Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3319-3323.	1.5	20
188	Spin injection and magnetoresistance in MoS ₂ -based tunnel junctions using Fe ₃ Si Heusler alloy electrodes. <i>Scientific Reports</i> , 2018, 8, 4779.	1.6	20
189	Hydrogen-Intercalated 2D Magnetic Bilayer: Controlled Magnetic Phase Transition and Half-Metallicity via Ferroelectric Switching. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 1800-1806.	4.0	20
190	Resonant magnetoresistance in organic spin valves (invited). <i>Journal of Applied Physics</i> , 2007, 101, 09B102.	1.1	19
191	Nonequilibrium Green's function study of Pd_4C_7 carbon nanotubes as hydrogen sensors. <i>Physical Review B</i> , 2009, 79, .	1.1	19
192	Quantum conductance of a single magnetic atom: An <i>ab initio</i> study. <i>Physical Review B</i> , 2010, 82, .	1.1	19
193	Origin of the transition voltage in gold "vacuum" gold atomic junctions. <i>Nanotechnology</i> , 2013, 24, 025203.	1.3	19
194	Proximity-induced topological state in graphene. <i>Physical Review B</i> , 2014, 90, .	1.1	19
195	Computational prediction of a two-dimensional semiconductor SnO_2 with negative Poisson's ratio and tunable magnetism by doping. <i>Physical Review B</i> , 2020, 102, .	1.1	19
196	Electric field response of strongly correlated one-dimensional metals: A Bethe ansatz density functional theory study. <i>Physical Review B</i> , 2010, 82, .	1.1	18
197	Magnetism and Antiferroelectricity in MgB_6 . <i>Physical Review Letters</i> , 2012, 108, 107205.	2.9	18
198	Spin transport properties of triarylamine-based nanowires. <i>Chemical Communications</i> , 2014, 50, 6626-6629.	2.2	18

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199	Substantial Band-Gap Tuning and a Strain-Controlled Semiconductor to Gapless/Band-Inverted Semimetal Transition in Rutile Lead/Stannic Dioxide. ACS Applied Materials & Interfaces, 2016, 8, 25667-25673.	4.0	18
200	Silver Tarnishing Mechanism Revealed by Molecular Dynamics Simulations. Angewandte Chemie - International Edition, 2019, 58, 6017-6021.	7.2	18
201	First-principles study of a Mn-doped In_2S_3 monolayer: Coexistence of ferromagnetism and ferroelectricity with robust half-metallicity and enhanced polarization. Physical Review B, 2020, 102, .	1.1	18
202	Pushing the limits of atomistic simulations towards ultra-high temperature: A machine-learning force field for ZrB2. Acta Materialia, 2020, 186, 467-474.	3.8	18
203	High-throughput bandstructure simulations of van der Waals hetero-bilayers formed by 1T and 2H monolayers. Npj 2D Materials and Applications, 2021, 5, .	3.9	18
204	The nanoscale structure of the Pt-water double layer under bias revealed. Electrochimica Acta, 2021, 391, 138875.	2.6	18
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