Stefano Sanvito

List of Publications by Year in descending order

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387 papers	23,892 citations	10956 71 h-index	8835 145 g-index
395 all docs	395 docs citations	395 times ranked	25029 citing authors

#	Article	IF	Citations
1	The rise of Nb-, Ta-, and Bi-based oxides/chalcogenides for photocatalytic applications. International Journal of Hydrogen Energy, 2022, 47, 3358-3370.	3.8	6
2	DFT-NEGF Simulation Study of Co₂FeAl-MgO-Co₂FeAl Magnetic Tunnel Junctions Under Biaxial Strain. IEEE Transactions on Magnetics, 2022, 58, 1-6.	1.2	1
3	Conservation of angular momentum in ultrafast spin dynamics. Physical Review B, 2022, 105, .	1.1	3
4	Complex band structure with non-orthogonal basis set: analytical properties and implementation in the SIESTA code. Journal of Physics Condensed Matter, 2022, 34, 105501.	0.7	2
5	Hydrogen-Intercalated 2D Magnetic Bilayer: Controlled Magnetic Phase Transition and Half-Metallicity via Ferroelectric Switching. ACS Applied Materials & Interfaces, 2022, 14, 1800-1806.	4.0	20
6	Fe- and Co-based magnetic tunnel junctions with AlN and ZnO spacers. Physical Review B, 2022, 105, .	1.1	3
7	Spectral neighbor representation for vector fields: Machine learning potentials including spin. Physical Review B, 2022, 105, .	1.1	9
8	Local inversion of the chemical environment representations. Physical Review B, 2022, 106, .	1.1	2
9	Prediction of room-temperature ferromagnetism and large perpendicular magnetic anisotropy in a planar hypercoordinate FeB₃monolayer. Nanoscale Horizons, 2021, 6, 43-48.	4.1	50
10	First-principles prediction of polar half-metallicity and out-of-plane piezoelectricity in two-dimensional quintuple layered cobalt selenide. Journal of Materials Chemistry C, 2021, 9, 12046-12050.	2.7	11
11	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
12	High-Performance Spin Filters Based on 1,2,4,5-Tetrahydroxybenzene Molecules Attached to Bulk Nickel Electrodes. Journal of Physical Chemistry C, 2021, 125, 6945-6953.	1.5	14
13	Spin transfer torque in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mn</mml:mi><mml:mn>3</mml:mn></m -based ferrimagnetic tunnel junctions from first principles. Physical Review B, 2021, 103, .	1.1	6
14	Data-driven enhancement of cubic phase stability in mixed-cation perovskites. Machine Learning: Science and Technology, 2021, 2, 025030.	2.4	17
15	Machine-learning semilocal density functional theory for many-body lattice models at zero and finite temperature. Physical Review B, 2021, 103, .	1.1	0
16	Using Weakly Supervised Deep Learning to Classify and Segment Singleâ€Molecule Breakâ€Junction Conductance Traces. ChemPhysChem, 2021, 22, 2107-2114.	1.0	4
17	Prediction of the two-dimensional Janus ferrovalley material LaBrI. Physical Review B, 2021, 104, .	1.1	49
18	In Situ Tuning of the Charge-Carrier Polarity in Imidazole-Linked Single-Molecule Junctions. Journal of Physical Chemistry Letters, 2021, 12, 7596-7604.	2.1	6

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19	Reactivity of transition-metal alloys to oxygen and sulfur. Physical Review Materials, 2021, 5, .	0.9	1
20	Purely one-dimensional ferroelectricity and antiferroelectricity from van der Waals niobium oxide trihalides. Npj Computational Materials, 2021, 7, .	3.5	14
21	The nanoscale structure of the Pt-water double layer under bias revealed. Electrochimica Acta, 2021, 391, 138875.	2.6	18
22	Atomistic simulations of surface reactions in ultra-high-temperature ceramics: O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e701" altimg="si64.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>, H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e709" altimg="si64.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:ms	3.1	4
23	Effect of a ferromagnetic STM cobalt tip on a single Co-phthalocyanine molecule adsorbed on a ferromagnetic substrate. Physics Open, 2021, 9, 100088.	0.7	1
24	Interfacing 2D VS2 with Janus MoSSe: Antiferromagnetic electric polarization and charge transfer driven Half-metallicity. Applied Surface Science, 2021, 570, 151129.	3.1	4
25	First-principles study of a Mn-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:m monolayer: Coexistence of ferromagnetism and ferroelectricity with robust half-metallicity and enhanced polarization. Physical Review B, 2020, 102, .	1.1	18
26	The Limit of Spin Lifetime in Solid-State Electronic Spins. Journal of Physical Chemistry Letters, 2020, 11, 6273-6278.	2.1	44
27	Improving stability of organometallic-halide perovskite solar cells using exfoliation two-dimensional molybdenum chalcogenides. Npj 2D Materials and Applications, 2020, 4, .	3.9	49
28	Photovoltage from ferroelectric domain walls in BiFeO3. Physical Review B, 2020, 102, .	1.1	8
29	Computational prediction of a two-dimensional semiconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SnO</mml:mi><mml:mn>2</mml:mn></m with negative Poisson's ratio and tunable magnetism by doping. Physical Review B, 2020, 102, .	1.1	19
30	Multiple spinâ€“phonon relaxation pathways in a Kramer single-ion magnet. Journal of Chemical Physics, 2020, 153, 174113.	1.2	49
31	Neutral excitation density-functional theory: an efficient and variational first-principles method for simulating neutral excitations in molecules. Scientific Reports, 2020, 10, 8947.	1.6	13
32	The 2020 magnetism roadmap. Journal Physics D: Applied Physics, 2020, 53, 453001.	1.3	162
33	Edge superconductivity in multilayer WTe2 Josephson junction. National Science Review, 2020, 7, 1468-1475.	4.6	22
34	Machine Learning Accelerated Recovery of the Cubic Structure in Mixed-Cation Perovskite Thin Films. Chemistry of Materials, 2020, 32, 2998-3006.	3.2	42
35	Importance of structural deformation features in the prediction of hybrid perovskite bandgaps. Computational Materials Science, 2020, 184, 109858.	1.4	22
36	Surfing Multiple Conformation-Property Landscapes via Machine Learning: Designing Single-Ion Magnetic Anisotropy. Journal of Physical Chemistry C, 2020, 124, 5802-5806.	1.5	22

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37	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
38	First-Principles Study of Electromigration in the Metallic Liquid State of GeTe and Sb₂Te₃ Phase-Change Compounds. Journal of Physical Chemistry C, 2020, 124, 9599-9603.	1.5	7
39	Electric-controlled half-metallicity in magnetic van der Waals heterobilayer. Journal of Materials Chemistry C, 2020, 8, 7034-7040.	2.7	29
40	Unveiling phonons in a molecular qubit with four-dimensional inelastic neutron scattering and density functional theory. Nature Communications, 2020, 11, 1751.	5.8	43
41	Electric field modulation of magnetism in ferrimagnetic Heusler heterostructures. Physical Review B, 2020, 101, .	1.1	24
42	Time-Dependent Density Functional Theory for Spin Dynamics. , 2020, , 841-866.		3
43	Machine Learning and High-Throughput Approaches to Magnetism. , 2020, , 351-373.		2
44	Ferroelectric control of electron half-metallicity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>A</mml:mi></mml:math> -type antiferromagnets and its application to nonvolatile memory devices. Physical Review B, 2020, 102, .	1.1	23
45	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
46	Theoretical investigation of the structural, elastic, electronic, and dielectric properties of alkali-metal-based bismuth ternary chalcogenides. Physical Review Materials, 2020, 4, .	0.9	7
47	Synthesis of centimeter-size free-standing perovskite nanosheets from single-crystal lead bromide for optoelectronic devices. Scientific Reports, 2019, 9, 11738.	1.6	9
48	Selfâ€Assembly of Atomically Thin Chiral Copper Heterostructures Templated by Black Phosphorus. Advanced Functional Materials, 2019, 29, 1903120.	7.8	9
49	First-Principles Investigation of Spinâ€“Phonon Coupling in Vanadium-Based Molecular Spin Quantum Bits. Inorganic Chemistry, 2019, 58, 10260-10268.	1.9	59
50	Learn-and-Match Molecular Cations for Perovskites. Journal of Physical Chemistry A, 2019, 123, 7323-7334.	1.1	28
51	How do phonons relax molecular spins?. Science Advances, 2019, 5, eaax7163.	4.7	74
52	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
53	Dirac-cone induced gating enhancement in single-molecule field-effect transistors. Nanoscale, 2019, 11, 13117-13125.	2.8	11
54	A unified picture of the covalent bond within quantum-accurate force fields: From organic molecules to metallic complexesâ€™ reactivity. Science Advances, 2019, 5, eaaw2210.	4.7	33

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55	Electronic spin-spin decoherence contribution in molecular qubits by quantum unitary spin dynamics. Journal of Magnetism and Magnetic Materials, 2019, 487, 165325.	1.0	9
56	Shaping and Storing Magnetic Data Using Pulsed Plasmonic Nanoheating and Spin-Transfer Torque. ACS Photonics, 2019, 6, 1524-1532.	3.2	9
57	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0
58	Ultrahigh conductivity in Weyl semimetal NbAs nanobelts. Nature Materials, 2019, 18, 482-488.	13.3	68
59	Silver Tarnishing Mechanism Revealed by Molecular Dynamics Simulations. Angewandte Chemie - International Edition, 2019, 58, 6017-6021.	7.2	18
60	Impurity band magnetism in organic semiconductors. Physical Review B, 2019, 99, .	1.1	5
61	Silver Tarnishing Mechanism Revealed by Molecular Dynamics Simulations. Angewandte Chemie, 2019, 131, 6078-6082.	1.6	8
62	Enhancing the electronic dimensionality of hybrid organicâ€“inorganic frameworks by hydrogen bonded molecular cations. Materials Horizons, 2019, 6, 1187-1196.	6.4	4
63	Machine learning density functional theory for the Hubbard model. Physical Review B, 2019, 99, .	1.1	29
64	Role of longitudinal fluctuations in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">L</mml:mi><mml:msub><mml:mn>1</mml:mn><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math FePt. Physical Review B, 2019, 100, .	1.1	5
65	Quantum Hall effect based on Weyl orbits in Cd3As2. Nature, 2019, 565, 331-336.	13.7	194
66	Nontrivial spatial dependence of the spin torques in L10 FePt-based tunneling junctions. Physical Review B, 2019, 99, .	1.1	3
67	First-Principles Prediction of a Room-Temperature Ferromagnetic Janus VSSe Monolayer with Piezoelectricity, Ferroelasticity, and Large Valley Polarization. Nano Letters, 2019, 19, 1366-1370.	4.5	292
68	Materials informatics. Journal of Intelligent Manufacturing, 2019, 30, 2307-2326.	4.4	90
69	Interface engineering of graphene nanosheet reinforced <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">ZrB</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> composites by tuning surface contacts. Physical Review Materials, 2019, 3, .	0.9	4
70	Predicting the Curie temperature of ferromagnets using machine learning. Physical Review Materials, 2019, 3, .	0.9	49
71	Interlayer dielectric function of a type-II van der Waals semiconductor: The <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>HfS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math heterobilayer. Physical Review Materials, 2019, 3, .	0.9	5
72	Proposal for a Dual Spin Filter Based on [VO(C₃S₄O)₂]^{2â€“}. Journal of Physical Chemistry C, 2018, 122, 6417-6421.	1.5	6

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73	Searching for Photoactive Polymorphs of CsNbQ₃ (Q = O, S, Se, Te) with Enhanced Optical Properties and Intrinsic Thermodynamic Stabilities. Journal of Physical Chemistry C, 2018, 122, 8814-8821.	1.5	11
74	Firstâ€principles investigation of the thermodynamic stability of MB₂ materials surfaces (MÂ=ÂTi/Zr/Hf). Journal of the American Ceramic Society, 2018, 101, 4118-4127.	1.9	9
75	A simple descriptor for energetics at fcc-bcc metal interfaces. Materials and Design, 2018, 142, 158-165.	3.3	15
76	Cr doping induced negative transverse magnetoresistance in Cd3As2 thin films. Physical Review B, 2018, 97, .	1.1	11
77	Electronâ€“Phonon Coupling and Polaron Mobility in Hybrid Perovskites from First Principles. Journal of Physical Chemistry C, 2018, 122, 1361-1366.	1.5	29
78	Ab initiosurface properties of Agâ€“Sn alloys: implications for lead-free soldering. Physical Chemistry Chemical Physics, 2018, 20, 4277-4286.	1.3	6
79	Spin injection and magnetoresistance in MoS2-based tunnel junctions using Fe3Si Heusler alloy electrodes. Scientific Reports, 2018, 8, 4779.	1.6	20
80	Computational investigation of label free detection of biomolecules based on armchair graphene nanoribbon. Sensors and Actuators B: Chemical, 2018, 255, 1276-1284.	4.0	9
81	Elucidating the Impact of Chalcogen Content on the Photovoltaic Properties of Oxychalcogenide Perovskites: NaMO_{3â^’x}Q_x (M=Nb, Ta; Q=S, Se, Te). ChemPhysChem, 2018, 19, 703-714.	1.0	17
82	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
83	Electron trapping by neutral pristine ferroelectric domain walls in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub><m Physical Review B, 2018, 98, .	1.1	11
84	Time-Dependent Density Functional Theory for Spin Dynamics. , 2018, , 1-26.		2
85	Spin-phonon coupling parameters from maximally localized Wannier functions and first-principles electronic structure: Single-crystal durene. Physical Review B, 2018, 98, .	1.1	5
86	Machine Learning and High-Throughput Approaches to Magnetism. , 2018, , 1-23.		3
87	AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. Journal of Chemical Information and Modeling, 2018, 58, 2477-2490.	2.5	69
88	Wannier-function-based constrained DFT with nonorthogonality-correcting Pulay forces in application to the reorganization effects in graphene-adsorbed pentacene. Physical Review B, 2018, 97, .	1.1	4
89	Effect of molecular conformations on the electronic transport in oxygen-substituted alkanethiol molecular junctions. Journal of Chemical Physics, 2018, 148, 184703.	1.2	5
90	Search for alternative magnetic tunnel junctions based on all-Heusler stacks. Physical Review B, 2018, 98, .	1.1	12

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91	Inducing Strong Superconductivity in WTe₂ by a Proximity Effect. ACS Nano, 2018, 12, 7185-7196.	7.3	48
92	Solar Cell Materials by Design: Hybrid Pyroxene Cornerâ€Sharing VO₄ Tetrahedral Chains. ChemSusChem, 2017, 10, 1931-1942.	3.6	10
93	Spin-orbit Hamiltonian for organic crystals from first-principles electronic structure and Wannier functions. Physical Review B, 2017, 95, .	1.1	7
94	Accelerated discovery of new magnets in the Heusler alloy family. Science Advances, 2017, 3, e1602241.	4.7	197
95	Theoretical Evaluation of [VIV(Î±-C3S5)3]2â€“as Nuclear-Spin-Sensitive Single-Molecule Spin Transistor. Journal of Physical Chemistry Letters, 2017, 8, 3056-3060.	2.1	14
96	Spin-Polarized Tunneling through Chemical Vapor Deposited Multilayer Molybdenum Disulfide. ACS Nano, 2017, 11, 6389-6395.	7.3	53
97	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>G junctions. Physical Review B, 2017, 95, .	1.1	31
98	Evolution of Weyl orbit and quantum Hall effect in Dirac semimetal Cd3As2. Nature Communications, 2017, 8, 1272.	5.8	118
99	Strain-induced Weyl and Dirac states and direct-indirect gap transitions in group-V materials. 2D Materials, 2017, 4, 045018.	2.0	22
100	Ultrafast demagnetizing fields from first principles. Physical Review B, 2017, 95, .	1.1	14
101	Evidence for pressure-induced node-pair annihilation in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">d</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal"></mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physi	1.1	14
102	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
103	An in situ and ex situ TEM study into the oxidation of titanium (IV) sulphide. Npj 2D Materials and Applications, 2017, 1, .	3.9	21
104	Intra-molecular origin of the spin-phonon coupling in slow-relaxing molecular magnets. Chemical Science, 2017, 8, 6051-6059.	3.7	160
105	The low-bias conducting mechanism of single-molecule junctions constructed with methylsulfide linker groups and gold electrodes. Journal of Chemical Physics, 2017, 147, 054702.	1.2	10
106	Ab initio dynamical exchange interactions in frustrated antiferromagnets. Physical Review B, 2017, 96, .	1.1	9
107	Multiscale modeling of current-induced switching in magnetic tunnel junctions using ab initio spin-transfer torques. Physical Review B, 2017, 96, .	1.1	24
108	Tailoring the Polarity of Charge Carriers in Grapheneâ€“Porphineâ€“Graphene Molecular Junctions through Linkage Motifs. Journal of Physical Chemistry C, 2017, 121, 27344-27350.	1.5	14

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109	First-Principles Prediction of Spin-Polarized Multiple Dirac Rings in Manganese Fluoride. Physical Review Letters, 2017, 119, 016403.	2.9	84
110	Resistive switching mechanism of GeTeâ€“Sb₂Te₃ interfacial phase change memory and topological properties of embedded two-dimensional states. Nanoscale, 2017, 9, 9386-9395.	2.8	36
111	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> as barriers in magnetic tunneling junctions. Physical Review B, 2017, 95, .	1.1	8
112	Influence of the dipolar interactions on the relative stability in spin crossover systems. Journal of Computational Chemistry, 2017, 38, 224-227.	1.5	3
113	The role of anharmonic phonons in under-barrier spin relaxation of single molecule magnets. Nature Communications, 2017, 8, 14620.	5.8	319
114	Quantitative Interpretation of the Lowâ€Bias Conductance of Auâ€“Mesityleneâ€“Au Molecular Junctions Formed from Mesitylene Monolayers. ChemPhysChem, 2016, 17, 2272-2277.	1.0	3
115	Effects of the molecule-electrode interface on the low-bias conductance of Cuâ€“H2â€“Cu single-molecule junctions. Journal of Chemical Physics, 2016, 145, 044701.	1.2	5
116	Cu-metalated carbyne acting as a promising molecular wire. Journal of Chemical Physics, 2016, 145, 244702.	1.2	5
117	Raman characterization of platinum diselenide thin films. 2D Materials, 2016, 3, 021004.	2.0	172
118	Current-induced changes of migration energy barriers in graphene and carbon nanotubes. Nanoscale, 2016, 8, 10310-10315.	2.8	3
119	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
120	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
121	Role of spin-orbit interaction in the ultrafast demagnetization of small iron clusters. Physical Review B, 2016, 94, .	1.1	22
122	Observation of quasi-two-dimensional Dirac fermions in ZrTe5. NPG Asia Materials, 2016, 8, e325-e325.	3.8	51
123	Persistent current and Drude weight of one-dimensional interacting fermions on imperfect ring from current lattice density functional theory. Journal of Physics Condensed Matter, 2016, 28, 445601.	0.7	1
124	Current-induced phonon renormalization in molecular junctions. Physical Review B, 2016, 94, .	1.1	10
125	Vertical Single-Crystalline Organic Nanowires on Graphene: Solution-Phase Epitaxy and Optical Microcavities. Nano Letters, 2016, 16, 4754-4762.	4.5	24
126	Designing a fully compensated half-metallic ferrimagnet. Physical Review B, 2016, 93, .	1.1	34

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127	Fundamental gap of molecular crystals via constrained density functional theory. Physical Review B, 2016, 93, .	1.1	13
128	Exploring the cation dynamics in lead-bromide hybrid perovskites. Physical Review B, 2016, 93, .	1.1	40
129	Charge transfer energies of benzene physisorbed on a graphene sheet from constrained density functional theory. Physical Review B, 2016, 93, .	1.1	13
130	Origin of the periodic structure in the conductance curve of gold nanojunctions in hydrogen environment. Physical Review B, 2016, 93, .	1.1	1
131	Effects of molecular dipole orientation on the exciton binding energy of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CH</mml:mi><mml:mn>3</mml:mn></mml: Physical Review B, 2016, 94, .	1.1	7
132	Zeeman splitting and dynamical mass generation in Dirac semimetal ZrTe5. Nature Communications, 2016, 7, 12516.	5.8	149
133	Dimensionality-driven phonon softening and incipient charge density wave instability in TiS ₂. Europhysics Letters, 2016, 115, 47001.	0.7	43
134	Charge and spin transport in single and packed ruthenium-terpyridine molecular devices: Insight from first-principles calculations. Scientific Reports, 2016, 6, 31856.	1.6	5
135	Tunneling magnetoresistance in Si nanowires. New Journal of Physics, 2016, 18, 113024.	1.2	4
136	Dynamic spin filtering at the Co/Alq3 interface mediated by weakly coupled second layer molecules. Nature Communications, 2016, 7, 12668.	5.8	55
137	Predicting Single-Layer Technetium Dichalcogenides (TcX₂, X = S, Se) with Promising Applications in Photovoltaics and Photocatalysis. ACS Applied Materials & Interfaces, 2016, 8, 5385-5392.	4.0	100
138	Revisiting the inelastic electron tunneling spectroscopy of single hydrogen atom adsorbed on the Cu(100) surface. Journal of Chemical Physics, 2015, 143, 234709.	1.2	4
139	Electronic Properties and Chemical Reactivity of TiS₂ Nanoflakes. Journal of Physical Chemistry C, 2015, 119, 15707-15715.	1.5	47
140	Charge carrier mobility in hybrid halide perovskites. Scientific Reports, 2015, 5, 12746.	1.6	294
141	Electronic Transport as a Driver for Self-Interaction-Corrected Methods. Advances in Atomic, Molecular and Optical Physics, 2015, 64, 29-86.	2.3	7
142	Spin-Valve Effect in NiFe/MoS₂/NiFe Junctions. Nano Letters, 2015, 15, 5261-5267.	4.5	135
143	First-principles investigation on the electronic efficiency and binding energy of the contacts formed by graphene and poly-aromatic hydrocarbon anchoring groups. Journal of Chemical Physics, 2015, 142, 164701.	1.2	8
144	Single atom anisotropic magnetoresistance on a topological insulator surface. New Journal of Physics, 2015, 17, 033021.	1.2	7

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145	Vibron-assisted spin relaxation at a metal/organic interface. Physical Review B, 2015, 91, .	1.1	6
146	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.	0.9	31
147	Revealing the role of organic cations in hybrid halide perovskite CH3NH3PbI3. Nature Communications, 2015, 6, 7026.	5.8	564
148	Basal-Plane Functionalization of Chemically Exfoliated Molybdenum Disulfide by Diazonium Salts. ACS Nano, 2015, 9, 6018-6030.	7.3	293
149	Single-Atom Based Coherent Quantum Interference Device Structure. Nano Letters, 2015, 15, 2881-2886.	4.5	10
150	Mechanism of H₂O-Induced Conductance Changes in AuCl₄-Functionalized CNTs. Journal of Physical Chemistry C, 2015, 119, 9568-9573.	1.5	5
151	The image charge effect and vibron-assisted processes in Coulomb blockade transport: a first principles approach. Nanoscale, 2015, 7, 19231-19240.	2.8	8
152	Controlling the Spin Texture of Topological Insulators by Rational Design of Organic Molecules. Nano Letters, 2015, 15, 6022-6029.	4.5	37
153	Liquid exfoliation of solvent-stabilized few-layer black phosphorus for applications beyond electronics. Nature Communications, 2015, 6, 8563.	5.8	921
154	Gate-tunable quantum oscillations in ambipolar Cd3As2 thin films. NPG Asia Materials, 2015, 7, e221-e221.	3.8	68
155	Ultrafast Non-local Spin Dynamics in Metallic Bi-Layers by Linear and Non-linear Magneto-Optics. Springer Proceedings in Physics, 2015, , 34-36.	0.1	2
156	Microscopic origin of the 1.3 G0 conductance observed in oxygen-doped silver quantum point contacts. Journal of Chemical Physics, 2014, 141, 194702.	1.2	3
157	First principles study of the structural, electronic, and transport properties of triarylamine-based nanowires. Journal of Chemical Physics, 2014, 140, 074301.	1.2	11
158	Transition voltages of vacuum-spaced and molecular junctions with Ag and Pt electrodes. Journal of Chemical Physics, 2014, 141, 014707.	1.2	7
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