Stefano Sanvito

List of Publications by Citations

371 papers	19,551 citations	66 h-index	131 g-index
395 ext. papers	21,868 ext. citations	6.1 avg, IF	7.28 L-index

#	Paper	IF	Citations
371	The high-throughput highway to computational materials design. *Nature Materials*, **2013**, 12, 191-201	27	1165
370	Towards molecular spintronics. *Nature Materials*, **2005**, 4, 335-9	27	1096
369	Molecular spintronics. *Chemical Society Reviews*, **2011**, 40, 3336-55	58.5	897
368	Liquid exfoliation of solvent-stabilized few-layer black phosphorus for applications beyond electronics. *Nature Communications*, **2015**, 6, 8563	17.4	764
367	AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. *Computational Materials Science*, **2012**, 58, 227-235	3.2	583
366	Spin and molecular electronics in atomically generated orbital landscapes. *Physical Review B*, **2006**, 73,	3.3	551
365	Solvent exfoliation of transition metal dichalcogenides: dispersibility of exfoliated nanosheets varies only weakly between compounds. *ACS Nano*, **2012**, 6, 3468-80	16.7	535
364	Hybrid graphene and graphitic carbon nitride nanocomposite: gap opening, electron-hole puddle, interfacial charge transfer, and enhanced visible light response. *Journal of the American Chemical Society*, **2012**, 134, 4393-7	16.4	490
363	Revealing the role of organic cations in hybrid halide perovskite CH3NH3PbI3. *Nature Communications*, **2015**, 6, 7026	17.4	489
362	Possible doping strategies for MoS2 monolayers: An ab initio study. *Physical Review B*, **2013**, 88,	3.3	416
361	Ferromagnetism driven by intrinsic point defects in HfO(2). *Physical Review Letters*, **2005**, 94, 217205	7.4	383
360	Self-interaction errors in density-functional calculations of electronic transport. *Physical Review Letters*, **2005**, 95, 146402	7.4	277
359	First-principles study of the origin and nature of ferromagnetism in Ga1□MnxAs. *Physical Review B*, **2001**, 63,	3.3	258
358	General Green□-function formalism for transport calculations with spd Hamiltonians and giant magnetoresistance in Co- and Ni-based magnetic multilayers. *Physical Review B*, **1999**, 59, 11936-11948	3.3	255
357	Algorithm for the construction of self-energies for electronic transport calculations based on singularity elimination and singular value decomposition. *Physical Review B*, **2008**, 78,	3.3	251
356	Origin of the n-type and p-type conductivity of MoS2 monolayers on a SiO2 substrate. *Physical Review B*, **2013**, 87,	3.3	235
355	First-principles prediction of metal-free magnetism and intrinsic half-metallicity in graphitic carbon nitride. *Physical Review Letters*, **2012**, 108, 197207	7.4	234

354	Basal-Plane Functionalization of Chemically Exfoliated Molybdenum Disulfide by Diazonium Salts. *ACS Nano*, **2015**, 9, 6018-30	16.7	232
353	Charge carrier mobility in hybrid halide perovskites. *Scientific Reports*, **2015**, 5, 12746	4.9	219
352	The role of anharmonic phonons in under-barrier spin relaxation of single molecule magnets. *Nature Communications*, **2017**, 8, 14620	17.4	215
351	Ground state of half-metallic zinc-blende MnAs. *Physical Review B*, **2000**, 62, 15553-15560	3.3	211
350	Mixed low-dimensional nanomaterial: 2D ultranarrow MoS2 inorganic nanoribbons encapsulated in quasi-1D carbon nanotubes. *Journal of the American Chemical Society*, **2010**, 132, 13840-7	16.4	188
349	Electric field effects on armchair MoS2 nanoribbons. *ACS Nano*, **2012**, 6, 4823-34	16.7	156
348	First-Principles Prediction of a Room-Temperature Ferromagnetic Janus VSSe Monolayer with Piezoelectricity, Ferroelasticity, and Large Valley Polarization. *Nano Letters*, **2019**, 19, 1366-1370	11.5	155
347	Fractional quantum conductance in carbon nanotubes. *Physical Review Letters*, **2000**, 84, 1974-7	7.4	150
346	Impurity-ion pair induced high-temperature ferromagnetism in Co-doped ZnO. *Physical Review B*, **2008**, 78,	3.3	144
345	Accelerated discovery of new magnets in the Heusler alloy family. *Science Advances*, **2017**, 3, e1602241	14.3	141
344	Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids. *Physical Review B*, **2007**, 75,	3.3	139
343	Raman characterization of platinum diselenide thin films. *2D Materials*, **2016**, 3, 021004	5.9	138
342	Electrostatic spin crossover effect in polar magnetic molecules. *Nature Materials*, **2009**, 8, 813-7	27	134
341	Electronic properties of bulk and thin film SrRuO3: Search for the metal-insulator transition. *Physical Review B*, **2008**, 78,	3.3	124
340	A spin of their own. *Nature Materials*, **2009**, 8, 693-5	27	123
339	Molecular-Spintronics: The Art of Driving Spin Through Molecules. *Journal of Computational and Theoretical Nanoscience*, **2006**, 3, 624-642	0.3	123
338	Magnetic semiconductors and half-metals. *Journal Physics D: Applied Physics*, **2004**, 37, 988-993	3	123
337	Efficient atomic self-interaction correction scheme for nonequilibrium quantum transport. *Physical Review Letters*, **2007**, 99, 056801	7.4	120

336	Novel one-dimensional organometallic half metals: vanadium-cyclopentadienyl, vanadium-cyclopentadienyl-benzene, and vanadium-anthracene wires. *Nano Letters*, **2008**, 8, 3640-4	11.5	116
335	Quantum Hall effect based on Weyl orbits in CdAs. *Nature*, **2019**, 565, 331-336	50.4	116
334	Effects of self-interaction corrections on the transport properties of phenyl-based molecular junctions. *Physical Review B*, **2008**, 77,	3.3	114
333	Predicting d0 magnetism: Self-interaction correction scheme. *Physical Review B*, **2008**, 78,	3.3	113
332	Intra-molecular origin of the spin-phonon coupling in slow-relaxing molecular magnets. *Chemical Science*, **2017**, 8, 6051-6059	9.4	112
331	Different origins of the ferromagnetic order in (Ga,Mn)As and (Ga,Mn)N. *Physical Review B*, **2004**, 70,	3.3	111
330	Zeeman splitting and dynamical mass generation in Dirac semimetal ZrTe5. *Nature Communications*, **2016**, 7, 12516	17.4	108
329	Spin-Valve Effect in NiFe/MoS2/NiFe Junctions. *Nano Letters*, **2015**, 15, 5261-7	11.5	102
328	Giant resistance change across the phase transition in spin-crossover molecules. *Physical Review Letters*, **2012**, 108, 217201	7.4	92
327	Influence of Quantum Confinement on the Electronic and Magnetic Properties of (Ga,Mn)As Diluted Magnetic Semiconductor. *Nano Letters*, **2002**, 2, 605-608	11.5	89
326	Molecular-Spintronics: The Art of Driving Spin Through Molecules. *Journal of Computational and Theoretical Nanoscience*, **2006**, 3, 624-642	0.3	89
325	Molecular Kondo chain. *Nano Letters*, **2012**, 12, 3174-9	11.5	83
324	Ab initio calculations of structural evolution and conductance of benzene-1,4-dithiol on gold leads. *ACS Nano*, **2011**, 5, 795-804	16.7	83
323	On-site approximation for spin□orbit coupling in linear combination of atomic orbitals density functional methods. *Journal of Physics Condensed Matter*, **2006**, 18, 7999-8013	1.8	80
322	Contact induced magnetism in carbon nanotubes. *Journal of Physics Condensed Matter*, **2004**, 16, L155-L161	1.8	80
321	Assessment of density functional theory for iron(II) molecules across the spin-crossover transition. *Journal of Chemical Physics*, **2012**, 137, 124303	3.9	79
320	Predicting Single-Layer Technetium Dichalcogenides (TcX□X = S, Se) with Promising Applications in Photovoltaics and Photocatalysis. *ACS Applied Materials & Interfaces*, **2016**, 8, 5385-92	9.5	78
319	Magnetic and electronic properties of D022-Mn3Ge (001) films. *Applied Physics Letters*, **2012**, 101, 132410	3.4	78

318	Density Functional Calculations for III1−xMnxV Diluted Ferromagnetic Semiconductors: A Review. *Journal of Superconductivity and Novel Magnetism*, **2002**, 15, 85-104		78
317	Evolution of Weyl orbit and quantum Hall effect in Dirac semimetal CdAs. *Nature Communications*, **2017**, 8, 1272	17.4	77
316	The 2020 magnetism roadmap. *Journal Physics D: Applied Physics*, **2020**, 53, 453001	3	77
315	Injecting and controlling spins in organic materials. *Journal of Materials Chemistry*, **2007**, 17, 4455		75
314	Effects induced by single and multiple dopants on the transport properties in zigzag-edged graphene nanoribbons. *Physical Review B*, **2009**, 80,	3.3	73
313	Site-specific order and magnetism in tetragonal Mn3Ga thin films. *Physical Review B*, **2013**, 87,	3.3	71
312	Variational pseudo-self-interaction-corrected density functional approach to the ab initio description of correlated solids and molecules. *Physical Review B*, **2011**, 84,	3.3	71
311	Electron doping and magnetic moment formation in N- and C-doped MgO. *Applied Physics Letters*, **2009**, 94, 252505	3.4	70
310	Efficient spin injection and giant magnetoresistance in Fe/MoS2/Fe junctions. *Physical Review B*, **2014**, 90,	3.3	67
309	Polaronic distortion and vacancy-induced magnetism in MgO. *Physical Review B*, **2010**, 81,	3.3	67
308	Molecular conduction: do time-dependent simulations tell you more than the Landauer approach?. *Journal of Chemical Physics*, **2006**, 124, 214708	3.9	67
307	Electric field control of valence tautomeric interconversion in cobalt dioxolene. *Physical Review Letters*, **2011**, 107, 047201	7.4	65
306	Functionalized Nanopore-Embedded Electrodes for Rapid DNA Sequencing. *Journal of Physical Chemistry C*, **2008**, 112, 3456-3459	3.8	65
305	Influence of the local As antisite distribution on ferromagnetism in (Ga, Mn)As. *Applied Physics Letters*, **2001**, 78, 3493-3495	3.4	65
304	First-Principles Prediction of Spin-Polarized Multiple Dirac Rings in Manganese Fluoride. *Physical Review Letters*, **2017**, 119, 016403	7.4	64
303	Gate-tunable quantum oscillations in ambipolar Cd3As2 thin films. *NPG Asia Materials*, **2015**, 7, e221-e221	10.3	60
302	Spin-filtering efficiency of ferrimagnetic spinels CoFe2O4 and NiFe2O4. *Physical Review B*, **2013**, 87,	3.3	59
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299	Ab initio calculation of the bias-dependent transport properties of Mn12 molecules. *Physical Review B*, **2009**, 80,	3.3	58
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290	Constrained-DFT method for accurate energy-level alignment of metal/molecule interfaces. *Physical Review B*, **2013**, 88,	3.3	46
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284	Ab initio transport theory for digital ferromagnetic heterostructures. *Physical Review Letters*, **2001**, 87, 267202	7.4	42
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281	Single-channel conductance of H2 molecules attached to platinum or palladium electrodes. *Physical Review B*, **2005**, 72,	3.3	41
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279	Ultrahigh conductivity in Weyl semimetal NbAs nanobelts. *Nature Materials*, **2019**, 18, 482-488	27	40
278	Finite-bias electronic transport of molecules in a water solution. *Physical Review B*, **2010**, 81,	3.3	40
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275	Exceptionally strong magnetism in the 4d perovskites RTcO3 (R=Ca, Sr, Ba). *Physical Review B*, **2011**, 83,	3.3	39
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272	Ab initio study of the magnetostructural properties of MnAs. *Physical Review B*, **2006**, 74,	3.3	39
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270	Unusual stacking variations in liquid-phase exfoliated transition metal dichalcogenides. *ACS Nano*, **2014**, 8, 3690-9	16.7	36
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265	How do phonons relax molecular spins?. *Science Advances*, **2019**, 5, eaax7163	14.3	34

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259	Dimensionality-driven phonon softening and incipient charge density wave instability in TiS 2. *Europhysics Letters*, **2016**, 115, 47001	1.6	31
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253	Exploring new approaches towards the formability of mixed-ion perovskites by DFT and machine learning. *Physical Chemistry Chemical Physics*, **2019**, 21, 1078-1088	3.6	29
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250	Structural Origins of Conductance Fluctuations in Gold-Thiolate Molecular Transport Junctions. *Journal of Physical Chemistry Letters*, **2013**, 4, 887-91	6.4	28
249	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	3.8	28
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245	Inducing Strong Superconductivity in WTe by a Proximity Effect. *ACS Nano*, **2018**, 12, 7185-7196	16.7	26
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241	First-principles calculation on the zero-bias conductance of a gold/1,4-diaminobenzene/gold molecular junction. *Nanotechnology*, **2007**, 18, 345203	3.4	25
240	Machine Learning Accelerated Recovery of the Cubic Structure in Mixed-Cation Perovskite Thin Films. *Chemistry of Materials*, **2020**, 32, 2998-3006	9.6	24
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235	Conceptual molecular quantum phase transistor based on first-principles quantum transport calculations. *Physical Review B*, **2008**, 78,	3.3	24
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232	Unveiling phonons in a molecular qubit with four-dimensional inelastic neutron scattering and density functional theory. *Nature Communications*, **2020**, 11, 1751	17.4	23
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230	Learn-and-Match Molecular Cations for Perovskites. *Journal of Physical Chemistry A*, **2019**, 123, 7323-7334	2.8	22
229	Effects of structural relaxation on calculations of the interface and transport properties of Fe/MgO(001) tunnel junctions. *Physical Review B*, **2009**, 79,	3.3	22

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227	Newtonian origin of the spin motive force in ferromagnetic atomic wires. *Physical Review B*, **2008**, 77,	3.3	22
226	Search for magnetoresistance in excess of 1000% in Ni point contacts: Density functional calculations. *Physical Review B*, **2007**, 76,	3.3	22
225	Lattice distortion effects on the magnetostructural phase transition of MnAs. *Physical Review Letters*, **2005**, 95, 077203	7.4	22
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223	Efficient conducting channels formed by the □stacking in single [2,2]paracyclophane molecules. *Journal of Chemical Physics*, **2012**, 136, 104701	3.9	21
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195	Strain-induced Weyl and Dirac states and direct-indirect gap transitions in group-V materials. *2D Materials*, **2017**, 4, 045018	5.9	16
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193	Charge Transport Properties of Durene Crystals from First-Principles. *Journal of Chemical Theory and Computation*, **2014**, 10, 4624-32	6.4	16

192	Origin of the p-Type Character of AuCl3 Functionalized Carbon Nanotubes. *Journal of Physical Chemistry C*, **2014**, 118, 3319-3323	3.8	16
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188	Magnetism and antiferroelectricity in MgB6. *Physical Review Letters*, **2012**, 108, 107205	7.4	16
187	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	9.5	16
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