# Stefano Sanvito

## List of Publications by Year in Descending Order

**Source:** https://exaly.com/author-pdf/2534209/stefano-sanvito-publications-by-year.pdf
**Version:** 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

| | | | |
|---|---|---|---|
| 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 | DFT-NEGF simulation study of Co2FeAl-MgO-Co2FeAl magnetic tunnel junctions under biaxial strain. *IEEE Transactions on Magnetics*, **2022**, 1-1 | 2 | |
| 370 | 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 | 3.8 | 4 |
| 369 | Data-driven enhancement of cubic phase stability in mixed-cation perovskites. *Machine Learning: Science and Technology*, **2021**, 2, 025030 | 5.1 | 3 |
| 368 | The rise of Nb-, Ta-, and Bi-based oxides/chalcogenides for photocatalytic applications. *International Journal of Hydrogen Energy*, **2021**, 47, 3358-3358 | 6.7 | 1 |
| 367 | Using Weakly Supervised Deep Learning to Classify and Segment Single-Molecule Break-Junction Conductance Traces. *ChemPhysChem*, **2021**, 22, 2107-2114 | 3.2 | 0 |
| 366 | Prediction of room-temperature ferromagnetism and large perpendicular magnetic anisotropy in a planar hypercoordinate FeB monolayer. *Nanoscale Horizons*, **2021**, 6, 43-48 | 10.8 | 19 |
| 365 | 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 | 7.1 | 2 |
| 364 | High-throughput bandstructure simulations of van der Waals hetero-bilayers formed by 1T and 2H monolayers. *Npj 2D Materials and Applications*, **2021**, 5, | 8.8 | 4 |
| 363 | Prediction of the two-dimensional Janus ferrovalley material LaBrI. *Physical Review B*, **2021**, 104, | 3.3 | 5 |
| 362 | In Situ Tuning of the Charge-Carrier Polarity in Imidazole-Linked Single-Molecule Junctions. *Journal of Physical Chemistry Letters*, **2021**, 12, 7596-7604 | 6.4 | 0 |
| 361 | Purely one-dimensional ferroelectricity and antiferroelectricity from van der Waals niobium oxide trihalides. *Npj Computational Materials*, **2021**, 7, | 10.9 | 2 |
| 360 | The nanoscale structure of the Pt-water double layer under bias revealed. *Electrochimica Acta*, **2021** , 391, 138875 | 6.7 | 8 |
| 359 | Atomistic simulations of surface reactions in ultra-high-temperature ceramics: O2, H2O and CO adsorption and dissociation on ZrB2(0001) surfaces. *Applied Surface Science*, **2021**, 566, 150622 | 6.7 | 1 |
| 358 | Effect of a ferromagnetic STM cobalt tip on a single Co-phthalocyanine molecule adsorbed on a ferromagnetic substrate. *Physics Open*, **2021**, 9, 100088 | 1.6 | |
| 357 | Interfacing 2D VS2 with Janus MoSSe: Antiferromagnetic electric polarization and charge transfer driven Half-metallicity. *Applied Surface Science*, **2021**, 570, 151129 | 6.7 | 1 |
| 356 | Computational prediction of a two-dimensional semiconductor SnO2 with negative Poisson's ratio and tunable magnetism by doping. *Physical Review B*, **2020**, 102, | 3.3 | 4 |
| 355 | Multiple spin-phonon relaxation pathways in a Kramer single-ion magnet. *Journal of Chemical Physics*, **2020**, 153, 174113 | 3.9 | 17 |

| | | | |
|---|---|---|---|
| 354 | Neutral excitation density-functional theory: an efficient and variational first-principles method for simulating neutral excitations in molecules. *Scientific Reports*, **2020**, 10, 8947 | 4.9 | 9 |
| 353 | The 2020 magnetism roadmap. *Journal Physics D: Applied Physics*, **2020**, 53, 453001 | 3 | 77 |
| 352 | Edge superconductivity in multilayer WTe Josephson junction. *National Science Review*, **2020**, 7, 1468-1475 | 15.8 | 10 |
| 351 | Machine Learning Accelerated Recovery of the Cubic Structure in Mixed-Cation Perovskite Thin Films. *Chemistry of Materials*, **2020**, 32, 2998-3006 | 9.6 | 24 |
| 350 | Importance of structural deformation features in the prediction of hybrid perovskite bandgaps. *Computational Materials Science*, **2020**, 184, 109858 | 3.2 | 9 |
| 349 | Surfing Multiple Conformation-Property Landscapes via Machine Learning: Designing Single-Ion Magnetic Anisotropy. *Journal of Physical Chemistry C*, **2020**, 124, 5802-5806 | 3.8 | 11 |
| 348 | Pushing the limits of atomistic simulations towards ultra-high temperature: A machine-learning force field for ZrB2. *Acta Materialia*, **2020**, 186, 467-474 | 8.4 | 7 |
| 347 | 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 | 3.8 | 6 |
| 346 | Electric-controlled half-metallicity in magnetic van der Waals heterobilayer. *Journal of Materials Chemistry C*, **2020**, 8, 7034-7040 | 7.1 | 16 |
| 345 | Unveiling phonons in a molecular qubit with four-dimensional inelastic neutron scattering and density functional theory. *Nature Communications*, **2020**, 11, 1751 | 17.4 | 23 |
| 344 | Electric field modulation of magnetism in ferrimagnetic Heusler heterostructures. *Physical Review B*, **2020**, 101, | 3.3 | 11 |
| 343 | Ferroelectric control of electron half-metallicity in A-type antiferromagnets and its application to nonvolatile memory devices. *Physical Review B*, **2020**, 102, | 3.3 | 3 |
| 342 | Theoretical investigation of the structural, elastic, electronic, and dielectric properties of alkali-metal-based bismuth ternary chalcogenides. *Physical Review Materials*, **2020**, 4, | 3.2 | 4 |
| 341 | The AFLOW Fleet for Materials Discovery **2020**, 1785-1812 | | 1 |
| 340 | Time-Dependent Density Functional Theory for Spin Dynamics **2020**, 841-866 | | 2 |
| 339 | Machine Learning and High-Throughput Approaches to Magnetism **2020**, 351-373 | | 1 |
| 338 | First-principles study of a Mn-doped In2Se3 monolayer: Coexistence of ferromagnetism and ferroelectricity with robust half-metallicity and enhanced polarization. *Physical Review B*, **2020**, 102, | 3.3 | 10 |
| 337 | The Limit of Spin Lifetime in Solid-State Electronic Spins. *Journal of Physical Chemistry Letters*, **2020**, 11, 6273-6278 | 6.4 | 15 |

| | | | |
|---|---|---|---|
| 336 | Improving stability of organometallic-halide perovskite solar cells using exfoliation two-dimensional molybdenum chalcogenides. *Npj 2D Materials and Applications*, **2020**, 4, | 8.8 | 17 |
| 335 | Photovoltage from ferroelectric domain walls in BiFeO3. *Physical Review B*, **2020**, 102, | 3.3 | 1 |
| 334 | How do phonons relax molecular spins?. *Science Advances*, **2019**, 5, eaax7163 | 14.3 | 34 |
| 333 | 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 |
| 332 | Dirac-cone induced gating enhancement in single-molecule field-effect transistors. *Nanoscale*, **2019** , 11, 13117-13125 | 7.7 | 8 |
| 331 | A unified picture of the covalent bond within quantum-accurate force fields: From organic molecules to metallic complexes' reactivity. *Science Advances*, **2019**, 5, eaaw2210 | 14.3 | 14 |
| 330 | Electronic spin-spin decoherence contribution in molecular qubits by quantum unitary spin dynamics. *Journal of Magnetism and Magnetic Materials*, **2019**, 487, 165325 | 2.8 | 7 |
| 329 | Shaping and Storing Magnetic Data Using Pulsed Plasmonic Nanoheating and Spin-Transfer Torque. *ACS Photonics*, **2019**, 6, 1524-1532 | 6.3 | 4 |
| 328 | The AFLOW Fleet for Materials Discovery **2019**, 1-28 | | |
| 327 | Ultrahigh conductivity in Weyl semimetal NbAs nanobelts. *Nature Materials*, **2019**, 18, 482-488 | 27 | 40 |
| 326 | Silver Tarnishing Mechanism Revealed by Molecular Dynamics Simulations. *Angewandte Chemie - International Edition*, **2019**, 58, 6017-6021 | 16.4 | 11 |
| 325 | Impurity band magnetism in organic semiconductors. *Physical Review B*, **2019**, 99, | 3.3 | 4 |
| 324 | Silver Tarnishing Mechanism Revealed by Molecular Dynamics Simulations. *Angewandte Chemie*, **2019**, 131, 6078-6082 | 3.6 | 4 |
| 323 | Synthesis of centimeter-size free-standing perovskite nanosheets from single-crystal lead bromide for optoelectronic devices. *Scientific Reports*, **2019**, 9, 11738 | 4.9 | 7 |
| 322 | Self-Assembly of Atomically Thin Chiral Copper Heterostructures Templated by Black Phosphorus. *Advanced Functional Materials*, **2019**, 29, 1903120 | 15.6 | 7 |
| 321 | First-Principles Investigation of Spin-Phonon Coupling in Vanadium-Based Molecular Spin Quantum Bits. *Inorganic Chemistry*, **2019**, 58, 10260-10268 | 5.1 | 31 |
| 320 | Learn-and-Match Molecular Cations for Perovskites. *Journal of Physical Chemistry A*, **2019**, 123, 7323-7334 | 2.8 | 22 |
| 319 | Interface engineering of graphene nanosheet reinforced ZrB2 composites by tuning surface contacts. *Physical Review Materials*, **2019**, 3, | 3.2 | 2 |

| | | | |
|---|---|---|---|
| 318 | Predicting the Curie temperature of ferromagnets using machine learning. *Physical Review Materials*, **2019**, 3, | 3.2 | 26 |
| 317 | Interlayer dielectric function of a type-II van der Waals semiconductor: The HfS2/PtS2 heterobilayer. *Physical Review Materials*, **2019**, 3, | 3.2 | 4 |
| 316 | Molecular Spintronics **2019**, 359-382 | | |
| 315 | Enhancing the electronic dimensionality of hybrid organic□inorganic frameworks by hydrogen bonded molecular cations. *Materials Horizons*, **2019**, 6, 1187-1196 | 14.4 | 3 |
| 314 | Machine learning density functional theory for the Hubbard model. *Physical Review B*, **2019**, 99, | 3.3 | 21 |
| 313 | Role of longitudinal fluctuations in L10 FePt. *Physical Review B*, **2019**, 100, | 3.3 | 2 |
| 312 | Quantum Hall effect based on Weyl orbits in CdAs. *Nature*, **2019**, 565, 331-336 | 50.4 | 116 |
| 311 | Nontrivial spatial dependence of the spin torques in L10 FePt-based tunneling junctions. *Physical Review B*, **2019**, 99, | 3.3 | 1 |
| 310 | 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 |
| 309 | Materials informatics. *Journal of Intelligent Manufacturing*, **2019**, 30, 2307-2326 | 6.7 | 50 |
| 308 | Proposal for a Dual Spin Filter Based on [VO(C3S4O)2]2□*Journal of Physical Chemistry C*, **2018**, 122, 6417-6421 | 3.8 | 5 |
| 307 | 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 | 3.8 | 8 |
| 306 | First-principles investigation of the thermodynamic stability of MB2 materials surfaces (M□=□Ti/Zr/Hf). *Journal of the American Ceramic Society*, **2018**, 101, 4118-4127 | 3.8 | 7 |
| 305 | A simple descriptor for energetics at fcc-bcc metal interfaces. *Materials and Design*, **2018**, 142, 158-165 | 8.1 | 9 |
| 304 | Cr doping induced negative transverse magnetoresistance in Cd3As2 thin films. *Physical Review B*, **2018**, 97, | 3.3 | 7 |
| 303 | Electron□Phonon Coupling and Polaron Mobility in Hybrid Perovskites from First Principles. *Journal of Physical Chemistry C*, **2018**, 122, 1361-1366 | 3.8 | 18 |
| 302 | Ab initio surface properties of Ag-Sn alloys: implications for lead-free soldering. *Physical Chemistry Chemical Physics*, **2018**, 20, 4277-4286 | 3.6 | 4 |
| 301 | Spin injection and magnetoresistance in MoS-based tunnel junctions using FeSi Heusler alloy electrodes. *Scientific Reports*, **2018**, 8, 4779 | 4.9 | 11 |

| | | | |
|---|---|---|---|
| 300 | Computational investigation of label free detection of biomolecules based on armchair graphene nanoribbon. *Sensors and Actuators B: Chemical*, **2018**, 255, 1276-1284 | 8.5 | 7 |
| 299 | Search for alternative magnetic tunnel junctions based on all-Heusler stacks. *Physical Review B*, **2018**, 98, | 3.3 | 8 |
| 298 | Inducing Strong Superconductivity in WTe by a Proximity Effect. *ACS Nano*, **2018**, 12, 7185-7196 | 16.7 | 26 |
| 297 | Elucidating the Impact of Chalcogen Content on the Photovoltaic Properties of Oxychalcogenide Perovkskites: NaMO Q (M=Nb, Ta; Q=S, Se, Te). *ChemPhysChem*, **2018**, 19, 703-714 | 3.2 | 12 |
| 296 | The AFLOW Fleet for Materials Discovery **2018**, 1-28 | | 9 |
| 295 | Electron trapping by neutral pristine ferroelectric domain walls in BiFeO3. *Physical Review B*, **2018**, 98, | 3.3 | 6 |
| 294 | Time-Dependent Density Functional Theory for Spin Dynamics **2018**, 1-26 | | 1 |
| 293 | Spin-phonon coupling parameters from maximally localized Wannier functions and first-principles electronic structure: Single-crystal durene. *Physical Review B*, **2018**, 98, | 3.3 | 4 |
| 292 | Machine Learning and High-Throughput Approaches to Magnetism **2018**, 1-23 | | 2 |
| 291 | AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. *Journal of Chemical Information and Modeling*, **2018**, 58, 2477-2490 | 6.1 | 43 |
| 290 | 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, | 3.3 | 4 |
| 289 | Effect of molecular conformations on the electronic transport in oxygen-substituted alkanethiol molecular junctions. *Journal of Chemical Physics*, **2018**, 148, 184703 | 3.9 | 3 |
| 288 | Solar Cell Materials by Design: Hybrid Pyroxene Corner-Sharing VO Tetrahedral Chains. *ChemSusChem*, **2017**, 10, 1931-1942 | 8.3 | 8 |
| 287 | Spin-orbit Hamiltonian for organic crystals from first-principles electronic structure and Wannier functions. *Physical Review B*, **2017**, 95, | 3.3 | 6 |
| 286 | Accelerated discovery of new magnets in the Heusler alloy family. *Science Advances*, **2017**, 3, e1602241 | 14.3 | 141 |
| 285 | Theoretical Evaluation of [V(□CS)] as Nuclear-Spin-Sensitive Single-Molecule Spin Transistor. *Journal of Physical Chemistry Letters*, **2017**, 8, 3056-3060 | 6.4 | 9 |
| 284 | Spin-Polarized Tunneling through Chemical Vapor Deposited Multilayer Molybdenum Disulfide. *ACS Nano*, **2017**, 11, 6389-6395 | 16.7 | 40 |
| 283 | First-principles spin-transfer torque in CuMnAs\|GaP\|CuMnAs junctions. *Physical Review B*, **2017**, 95, | 3.3 | 20 |

| | | | |
|---|---|---|---|
| 282 | Evolution of Weyl orbit and quantum Hall effect in Dirac semimetal CdAs. *Nature Communications*, **2017**, 8, 1272 | 17.4 | 77 |
| 281 | Strain-induced Weyl and Dirac states and direct-indirect gap transitions in group-V materials. *2D Materials*, **2017**, 4, 045018 | 5.9 | 16 |
| 280 | Ultrafast demagnetizing fields from first principles. *Physical Review B*, **2017**, 95, | 3.3 | 10 |
| 279 | Evidence for pressure-induced node-pair annihilation in Cd3As2. *Physical Review B*, **2017**, 96, | 3.3 | 7 |
| 278 | 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 | 7.4 | 58 |
| 277 | An in situ and ex situ TEM study into the oxidation of titanium (IV) sulphide. *Npj 2D Materials and Applications*, **2017**, 1, | 8.8 | 15 |
| 276 | Intra-molecular origin of the spin-phonon coupling in slow-relaxing molecular magnets. *Chemical Science*, **2017**, 8, 6051-6059 | 9.4 | 112 |
| 275 | The low-bias conducting mechanism of single-molecule junctions constructed with methylsulfide linker groups and gold electrodes. *Journal of Chemical Physics*, **2017**, 147, 054702 | 3.9 | 8 |
| 274 | Ab initio dynamical exchange interactions in frustrated antiferromagnets. *Physical Review B*, **2017**, 96, | 3.3 | 6 |
| 273 | Multiscale modeling of current-induced switching in magnetic tunnel junctions using ab initio spin-transfer torques. *Physical Review B*, **2017**, 96, | 3.3 | 16 |
| 272 | Tailoring the Polarity of Charge Carriers in Graphene□Porphine□Graphene Molecular Junctions through Linkage Motifs. *Journal of Physical Chemistry C*, **2017**, 121, 27344-27350 | 3.8 | 10 |
| 271 | First-Principles Prediction of Spin-Polarized Multiple Dirac Rings in Manganese Fluoride. *Physical Review Letters*, **2017**, 119, 016403 | 7.4 | 64 |
| 270 | Resistive switching mechanism of GeTe-SbTe interfacial phase change memory and topological properties of embedded two-dimensional states. *Nanoscale*, **2017**, 9, 9386-9395 | 7.7 | 32 |
| 269 | HfO2 and SiO2 as barriers in magnetic tunneling junctions. *Physical Review B*, **2017**, 95, | 3.3 | 2 |
| 268 | Influence of the dipolar interactions on the relative stability in spin crossover systems. *Journal of Computational Chemistry*, **2017**, 38, 224-227 | 3.5 | 2 |
| 267 | The role of anharmonic phonons in under-barrier spin relaxation of single molecule magnets. *Nature Communications*, **2017**, 8, 14620 | 17.4 | 215 |
| 266 | Observation of quasi-two-dimensional Dirac fermions in ZrTe5. *NPG Asia Materials*, **2016**, 8, e325-e325 | 10.3 | 41 |
| 265 | 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 | 1.8 | 1 |

| | | | |
|---|---|---|---|
| 264 | Current-induced phonon renormalization in molecular junctions. *Physical Review B*, **2016**, 94, | 3.3 | 8 |
| 263 | Vertical Single-Crystalline Organic Nanowires on Graphene: Solution-Phase Epitaxy and Optical Microcavities. *Nano Letters*, **2016**, 16, 4754-62 | 11.5 | 20 |
| 262 | Designing a fully compensated half-metallic ferrimagnet. *Physical Review B*, **2016**, 93, | 3.3 | 26 |
| 261 | Fundamental gap of molecular crystals via constrained density functional theory. *Physical Review B*, **2016**, 93, | 3.3 | 13 |
| 260 | Exploring the cation dynamics in lead-bromide hybrid perovskites. *Physical Review B*, **2016**, 93, | 3.3 | 35 |
| 259 | Charge transfer energies of benzene physisorbed on a graphene sheet from constrained density functional theory. *Physical Review B*, **2016**, 93, | 3.3 | 10 |
| 258 | Origin of the periodic structure in the conductance curve of gold nanojunctions in hydrogen environment. *Physical Review B*, **2016**, 93, | 3.3 | 1 |
| 257 | Effects of molecular dipole orientation on the exciton binding energy of CH3NH3PbI3. *Physical Review B*, **2016**, 94, | 3.3 | 6 |
| 256 | Zeeman splitting and dynamical mass generation in Dirac semimetal ZrTe5. *Nature Communications*, **2016**, 7, 12516 | 17.4 | 108 |
| 255 | Dimensionality-driven phonon softening and incipient charge density wave instability in TiS 2. *Europhysics Letters*, **2016**, 115, 47001 | 1.6 | 31 |
| 254 | Charge and spin transport in single and packed ruthenium-terpyridine molecular devices: Insight from first-principles calculations. *Scientific Reports*, **2016**, 6, 31856 | 4.9 | 4 |
| 253 | Tunneling magnetoresistance in Si nanowires. *New Journal of Physics*, **2016**, 18, 113024 | 2.9 | 0 |
| 252 | Dynamic spin filtering at the Co/Alq3 interface mediated by weakly coupled second layer molecules. *Nature Communications*, **2016**, 7, 12668 | 17.4 | 39 |
| 251 | 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 |
| 250 | The oxidation of gallium (II) sulphide **2016**, 528-529 | | |
| 249 | Quantitative Interpretation of the Low-Bias Conductance of Au-Mesitylene-Au Molecular Junctions Formed from Mesitylene Monolayers. *ChemPhysChem*, **2016**, 17, 2272-7 | 3.2 | 3 |
| 248 | Effects of the molecule-electrode interface on the low-bias conductance of Cu-H2-Cu single-molecule junctions. *Journal of Chemical Physics*, **2016**, 145, 044701 | 3.9 | 4 |
| 247 | Cu-metalated carbyne acting as a promising molecular wire. *Journal of Chemical Physics*, **2016**, 145, 244702 | 3.9 | 3 |

| | | | |
|---|---|---|---|
| 246 | Raman characterization of platinum diselenide thin films. *2D Materials*, **2016**, 3, 021004 | 5.9 | 138 |
| 245 | Current-induced changes of migration energy barriers in graphene and carbon nanotubes. *Nanoscale*, **2016**, 8, 10310-5 | 7.7 | 2 |
| 244 | 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 |
| 243 | Spin Transfer Torque: A Multiscale Picture **2016**, 91-132 | | 4 |
| 242 | Diffusion Monte Carlo Perspective on the Spin-State Energetics of [Fe(NCH)6](2.). *Journal of Chemical Theory and Computation*, **2016**, 12, 4233-41 | 6.4 | 22 |
| 241 | Role of spin-orbit interaction in the ultrafast demagnetization of small iron clusters. *Physical Review B*, **2016**, 94, | 3.3 | 14 |
| 240 | Charge carrier mobility in hybrid halide perovskites. *Scientific Reports*, **2015**, 5, 12746 | 4.9 | 219 |
| 239 | Electronic Transport as a Driver for Self-Interaction-Corrected Methods. *Advances in Atomic, Molecular and Optical Physics*, **2015**, 64, 29-86 | 1.7 | 6 |
| 238 | Spin-Valve Effect in NiFe/MoS2/NiFe Junctions. *Nano Letters*, **2015**, 15, 5261-7 | 11.5 | 102 |
| 237 | 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 | 3.9 | 6 |
| 236 | Single atom anisotropic magnetoresistance on a topological insulator surface. *New Journal of Physics*, **2015**, 17, 033021 | 2.9 | 6 |
| 235 | Vibron-assisted spin relaxation at a metal/organic interface. *Physical Review B*, **2015**, 91, | 3.3 | 4 |
| 234 | 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 | 2.1 | 28 |
| 233 | Revealing the role of organic cations in hybrid halide perovskite CH3NH3PbI3. *Nature Communications*, **2015**, 6, 7026 | 17.4 | 489 |
| 232 | Basal-Plane Functionalization of Chemically Exfoliated Molybdenum Disulfide by Diazonium Salts. *ACS Nano*, **2015**, 9, 6018-30 | 16.7 | 232 |
| 231 | Single-atom based coherent quantum interference device structure. *Nano Letters*, **2015**, 15, 2881-6 | 11.5 | 7 |
| 230 | Mechanism of H2O-Induced Conductance Changes in AuCl4-Functionalized CNTs. *Journal of Physical Chemistry C*, **2015**, 119, 9568-9573 | 3.8 | 5 |
| 229 | The image charge effect and vibron-assisted processes in Coulomb blockade transport: a first principles approach. *Nanoscale*, **2015**, 7, 19231-40 | 7.7 | 7 |

| | | | |
|---|---|---|---|
| 228 | Controlling the Spin Texture of Topological Insulators by Rational Design of Organic Molecules. *Nano Letters*, **2015**, 15, 6022-9 | 11.5 | 30 |
| 227 | Liquid exfoliation of solvent-stabilized few-layer black phosphorus for applications beyond electronics. *Nature Communications*, **2015**, 6, 8563 | 17.4 | 764 |
| 226 | A First Principle Study of the Massive TMR in Magnetic Tunnel Junction Using Fe3Al Heusler Alloy Electrodes and MgO Barrier. *Advanced Materials Research*, **2015**, 1101, 192-197 | 0.5 | 1 |
| 225 | Gate-tunable quantum oscillations in ambipolar Cd3As2 thin films. *NPG Asia Materials*, **2015**, 7, e221-e221 | 10.3 | 60 |
| 224 | Revisiting the inelastic electron tunneling spectroscopy of single hydrogen atom adsorbed on the Cu(100) surface. *Journal of Chemical Physics*, **2015**, 143, 234709 | 3.9 | 4 |
| 223 | Electronic Properties and Chemical Reactivity of TiS2 Nanoflakes. *Journal of Physical Chemistry C*, **2015**, 119, 15707-15715 | 3.8 | 37 |
| 222 | Ultrafast Non-local Spin Dynamics in Metallic Bi-Layers by Linear and Non-linear Magneto-Optics. *Springer Proceedings in Physics*, **2015**, 34-36 | 0.2 | 2 |
| 221 | Multiprobe quantum spin Hall bars. *European Physical Journal B*, **2014**, 87, 1 | 1.2 | 5 |
| 220 | Electronic and magnetic properties of the interface between metal-quinoline molecules and cobalt. *Physical Review B*, **2014**, 89, | 3.3 | 33 |
| 219 | Spin transport properties of triarylamine-based nanowires. *Chemical Communications*, **2014**, 50, 6626-9 | 5.8 | 15 |
| 218 | Molecular dynamics investigation of carbon nanotube junctions in non-aqueous solutions. *Journal of Materials Chemistry A*, **2014**, 2, 16498-16506 | 13 | 1 |
| 217 | Stretching of BDT-gold molecular junctions: thiol or thiolate termination?. *Nanoscale*, **2014**, 6, 14495-507 | 7.7 | 35 |
| 216 | Proximity-induced topological state in graphene. *Physical Review B*, **2014**, 90, | 3.3 | 17 |
| 215 | Charge Transport Properties of Durene Crystals from First-Principles. *Journal of Chemical Theory and Computation*, **2014**, 10, 4624-32 | 6.4 | 16 |
| 214 | Efficient spin injection and giant magnetoresistance in Fe/MoS2/Fe junctions. *Physical Review B*, **2014**, 90, | 3.3 | 67 |
| 213 | Electronic structure of metal quinoline molecules from G0W0 calculations. *Physical Review B*, **2014**, 89, | 3.3 | 11 |
| 212 | Origin of the p-Type Character of AuCl3 Functionalized Carbon Nanotubes. *Journal of Physical Chemistry C*, **2014**, 118, 3319-3323 | 3.8 | 16 |
| 211 | Unusual stacking variations in liquid-phase exfoliated transition metal dichalcogenides. *ACS Nano*, **2014**, 8, 3690-9 | 16.7 | 36 |

| | | | |
|---|---|---|---|
| 210 | Microscopic origin of the 1.3 G(0) conductance observed in oxygen-doped silver quantum point contacts. *Journal of Chemical Physics*, **2014**, 141, 194702 | 3.9 | 1 |
| 209 | First principles study of the structural, electronic, and transport properties of triarylamine-based nanowires. *Journal of Chemical Physics*, **2014**, 140, 074301 | 3.9 | 11 |
| 208 | Transition voltages of vacuum-spaced and molecular junctions with Ag and Pt electrodes. *Journal of Chemical Physics*, **2014**, 141, 014707 | 3.9 | 6 |
| 207 | Topological tuning in three-dimensional dirac semimetals. *Physical Review Letters*, **2014**, 113, 256403 | 7.4 | 45 |
| 206 | Microscopic mechanism of electron transfer through the hydrogen bonds between carboxylated alkanethiol molecules connected to gold electrodes. *Journal of Chemical Physics*, **2014**, 141, 174702 | 3.9 | 5 |
| 205 | Ab initio transport across bismuth selenide surface barriers. *Physical Review B*, **2014**, 90, | 3.3 | 12 |
| 204 | Tailoring highly conductive graphene nanoribbons from small polycyclic aromatic hydrocarbons: a computational study. *Journal of Physics Condensed Matter*, **2013**, 25, 275301 | 1.8 | 1 |
| 203 | Many-body quasiparticle spectrum of Co-doped ZnO: A GW perspective. *Physical Review B*, **2013**, 87, | 3.3 | 19 |
| 202 | Spin-polarized transport through single-molecule magnet Mn6 complexes. *Nanoscale*, **2013**, 5, 4751-7 | 7.7 | 16 |
| 201 | Structural and tunneling properties of Si nanowires. *Physical Review B*, **2013**, 88, | 3.3 | 4 |
| 200 | Spin-filtering efficiency of ferrimagnetic spinels CoFe2O4 and NiFe2O4. *Physical Review B*, **2013**, 87, | 3.3 | 59 |
| 199 | Structural Origins of Conductance Fluctuations in Gold-Thiolate Molecular Transport Junctions. *Journal of Physical Chemistry Letters*, **2013**, 4, 887-91 | 6.4 | 28 |
| 198 | Possible doping strategies for MoS2 monolayers: An ab initio study. *Physical Review B*, **2013**, 88, | 3.3 | 416 |
| 197 | Constrained-DFT method for accurate energy-level alignment of metal/molecule interfaces. *Physical Review B*, **2013**, 88, | 3.3 | 46 |
| 196 | The high-throughput highway to computational materials design. *Nature Materials*, **2013**, 12, 191-201 | 27 | 1165 |
| 195 | Time-dependent electron transport through a strongly correlated quantum dot: multiple-probe open-boundary conditions approach. *Journal of Physics Condensed Matter*, **2013**, 25, 105501 | 1.8 | 5 |
| 194 | Origin of the n-type and p-type conductivity of MoS2 monolayers on a SiO2 substrate. *Physical Review B*, **2013**, 87, | 3.3 | 235 |
| 193 | Origin of the half-metallic properties of graphitic carbon nitride in bulk and confined forms. *Journal of Materials Chemistry C*, **2013**, 1, 3655 | 7.1 | 9 |

| | | | |
|---|---|---|---|
| 192 | Atomistic simulations of highly conductive molecular transport junctions under realistic conditions. *Nanoscale*, **2013**, 5, 3654-9 | 7.7 | 30 |
| 191 | Ground state of a spin-crossover molecule calculated by diffusion Monte Carlo. *Physical Review B*, **2013**, 87, | 3.3 | 16 |
| 190 | Spin-pumping and inelastic electron tunneling spectroscopy in topological insulators. *Physical Review B*, **2013**, 87, | 3.3 | 6 |
| 189 | Origin of the transition voltage in gold-vacuum-gold atomic junctions. *Nanotechnology*, **2013**, 24, 025203 | 3.4 | 18 |
| 188 | Anomalous length dependence of the conductance of graphene nanoribbons with zigzag edges. *Journal of Chemical Physics*, **2013**, 138, 014704 | 3.9 | 2 |
| 187 | Quantitative interpretation of the transition voltages in gold-poly(phenylene) thiol-gold molecular junctions. *Journal of Chemical Physics*, **2013**, 139, 194703 | 3.9 | 6 |
| 186 | Hydrogen bonding as the origin of the switching behavior in dithiolated phenylene-vinylene oligomers. *Physical Review B*, **2013**, 88, | 3.3 | 4 |
| 185 | Site-specific order and magnetism in tetragonal Mn3Ga thin films. *Physical Review B*, **2013**, 87, | 3.3 | 71 |
| 184 | Ab initio theory for current-induced molecular switching: Melamine on Cu(001). *Physical Review B*, **2013**, 87, | 3.3 | 24 |
| 183 | Dynamical exchange interaction from time-dependent spin density functional theory. *Physical Review B*, **2013**, 88, | 3.3 | 7 |
| 182 | Spin-dependent electronic structure of the Co/Al(OP)3interface. *New Journal of Physics*, **2013**, 15, 113054 | 3.9 | 19 |
| 181 | Spin Inelastic Electron Spectroscopy for Single Magnetic Atoms **2013**, 471-492 | | |
| 180 | Gate controlled spin pumping at a quantum spin Hall edge. *Applied Physics Letters*, **2013**, 103, 142407 | 3.4 | 3 |
| 179 | Topological surface states scattering in antimony. *Physical Review B*, **2012**, 86, | 3.3 | 19 |
| 178 | Molecular Kondo chain. *Nano Letters*, **2012**, 12, 3174-9 | 11.5 | 83 |
| 177 | Electronic transport through EuO spin-filter tunnel junctions. *Physical Review B*, **2012**, 86, | 3.3 | 18 |
| 176 | Efficient conducting channels formed by the $\pi$-stacking in single [2,2]paracyclophane molecules. *Journal of Chemical Physics*, **2012**, 136, 104701 | 3.9 | 21 |
| 175 | Protocol for classical molecular dynamics simulations of nano-junctions in solution. *Journal of Applied Physics*, **2012**, 112, 083714 | 2.5 | |

| | | | |
|---|---|---|---|
| 174 | First Principles Study of Electron Tunneling through Ice. *Journal of Physical Chemistry C*, **2012**, 116, 22129-22138 | 3.8 | 83 |
| 173 | Andreev reflection in two-dimensional topological insulators with either conserved or broken time-reversal symmetry. *Physical Review B*, **2012**, 86, | 3.3 | 13 |
| 172 | AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. *Computational Materials Science*, **2012**, 58, 227-235 | 3.2 | 583 |
| 171 | Persistent current and Drude weight for the one-dimensional Hubbard model from current lattice density functional theory. *Journal of Physics Condensed Matter*, **2012**, 24, 055602 | 1.8 | 7 |
| 170 | Solvent exfoliation of transition metal dichalcogenides: dispersibility of exfoliated nanosheets varies only weakly between compounds. *ACS Nano*, **2012**, 6, 3468-80 | 16.7 | 535 |
| 169 | First principle investigation of transport properties of Lindqvist derivatives based molecular junction. *Journal of Molecular Graphics and Modelling*, **2012**, 38, 220-5 | 2.8 | 5 |
| 168 | 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 |
| 167 | Assessment of density functional theory for iron(II) molecules across the spin-crossover transition. *Journal of Chemical Physics*, **2012**, 137, 124303 | 3.9 | 79 |
| 166 | Giant resistance change across the phase transition in spin-crossover molecules. *Physical Review Letters*, **2012**, 108, 217201 | 7.4 | 92 |
| 165 | First-principles prediction of metal-free magnetism and intrinsic half-metallicity in graphitic carbon nitride. *Physical Review Letters*, **2012**, 108, 197207 | 7.4 | 234 |
| 164 | First-principles study of high-conductance DNA sequencing with carbon nanotube electrodes. *Physical Review B*, **2012**, 85, | 3.3 | 29 |
| 163 | Spectroscopic characterization of a single dangling bond on a bare Si(100)-c(4□2) surface for n- and p-type doping. *Physical Review B*, **2012**, 86, | 3.3 | 8 |
| 162 | Ge-based spin-photodiodes for room-temperature integrated detection of photon helicity. *Advanced Materials*, **2012**, 24, 3037-41 | 24 | 36 |
| 161 | Electric field effects on armchair MoS2 nanoribbons. *ACS Nano*, **2012**, 6, 4823-34 | 16.7 | 156 |
| 160 | Contact geometry and electronic transport properties of Ag□benzene□Ag molecular junctions. *Chemical Physics*, **2012**, 397, 82-86 | 2.3 | 5 |
| 159 | Effects of the covalent linker groups on the spin transport properties of single nickelocene molecules attached to single-walled carbon nanotubes. *Journal of Chemical Physics*, **2012**, 136, 194707 | 3.9 | 4 |
| 158 | Nucleobase adsorbed at graphene devices: Enhance bio-sensorics. *Applied Physics Letters*, **2012**, 100, 063101 | 3.4 | 40 |
| 157 | Anomalous length dependence of conductance of aromatic nanoribbons with amine anchoring groups. *Physical Review B*, **2012**, 86, | 3.3 | 3 |

| | | | |
|---|---|---|---|
| 156 | Bias asymmetry in the conductance profile of magnetic ions on surfaces probed by scanning tunneling microscopy. *Physical Review B*, **2012**, 86, | 3.3 | 6 |
| 155 | Quantum transport of Au-S-S-Au nanoscale junctions. *Applied Physics Letters*, **2012**, 100, 013113 | 3.4 | 14 |
| 154 | Magnetism and antiferroelectricity in MgB6. *Physical Review Letters*, **2012**, 108, 107205 | 7.4 | 16 |
| 153 | Coexistance of giant tunneling electroresistance and magnetoresistance in an all-oxide composite magnetic tunnel junction. *Physical Review Letters*, **2012**, 109, 226803 | 7.4 | 26 |
| 152 | Magnetic and electronic properties of D022-Mn3Ge (001) films. *Applied Physics Letters*, **2012**, 101, 132410 | 3.4 | 78 |
| 151 | Tailoring magnetoresistance at the atomic level: An ab initio study. *Physical Review B*, **2012**, 85, | 3.3 | 2 |
| 150 | Bias-dependent oscillatory electron transport of monatomic sulfur chains. *Applied Physics Letters*, **2012**, 100, 103110 | 3.4 | 14 |
| 149 | Persistent current and Drude weight for the one-dimensional Hubbard model from current lattice density functional theory. *Journal of Physics Condensed Matter*, **2012**, 24, 099601 | 1.8 | 3 |
| 148 | Exceptionally strong magnetism in the 4d perovskites RTcO3 (R=Ca, Sr, Ba). *Physical Review B*, **2011**, 83, | 3.3 | 39 |
| 147 | Electric field control of valence tautomeric interconversion in cobalt dioxolene. *Physical Review Letters*, **2011**, 107, 047201 | 7.4 | 65 |
| 146 | Organic spintronics: filtering spins with molecules. *Nature Materials*, **2011**, 10, 484-5 | 27 | 51 |
| 145 | Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods. *Physical Review B*, **2011**, 84, | 3.3 | 53 |
| 144 | Prediction of large bias-dependent magnetoresistance in all-oxide magnetic tunnel junctions with a ferroelectric barrier. *Physical Review B*, **2011**, 83, | 3.3 | 24 |
| 143 | Molecular spintronics. *Chemical Society Reviews*, **2011**, 40, 3336-55 | 58.5 | 897 |
| 142 | From zigzag to armchair: the energetic stability, electronic and magnetic properties of chiral graphene nanoribbons with hydrogen-terminated edges. *Journal of Physics Condensed Matter*, **2011**, 23, 425301 | 1.8 | 18 |
| 141 | From fused aromatics to graphene-like nanoribbons: The effects of multiple terminal groups, length and symmetric pathways on charge transport. *Physical Review B*, **2011**, 84, | 3.3 | 5 |
| 140 | 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 |
| 139 | Effects of edge chemistry doping on graphene nanoribbon mobility. *Surface Science*, **2011**, 605, 1643-1648 | 1.8 | 24 |

| | | | |
|---|---|---|---|
| 138 | The search for a spin crossover transition in small sized Ɛ-conjugated molecules: a Monte Carlo study. *Journal of Physics Condensed Matter*, **2011**, 23, 316001 | 1.8 | 2 |
| 137 | Scattered surface charge density: A tool for surface characterization. *Physical Review B*, **2011**, 84, | 3.3 | 7 |
| 136 | Perturbative approach to the Kondo effect in magnetic atoms on nonmagnetic substrates. *Physical Review B*, **2011**, 84, | 3.3 | 20 |
| 135 | Spin scattering and spin-polarized hybrid interface states at a metal-organic interface. *Physical Review B*, **2011**, 84, | 3.3 | 44 |
| 134 | Current-induced energy barrier suppression for electromigration from first principles. *Physical Review B*, **2011**, 84, | 3.3 | 22 |
| 133 | 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 |
| 132 | Comparison between s- and d-electron mediated transport in a photoswitching dithienylethene molecule using ab initio transport methods. *Physical Review B*, **2011**, 84, | 3.3 | 3 |
| 131 | Electrical control of spin dynamics in finite one-dimensional systems. *Physical Review B*, **2011**, 84, | 3.3 | 3 |
| 130 | Spin transport in higher n-acene molecules. *Physical Review B*, **2011**, 84, | 3.3 | 24 |
| 129 | Spin-flip inelastic electron tunneling spectroscopy in atomic chains. *Physical Review B*, **2011**, 84, | 3.3 | 21 |
| 128 | Spin transport properties of single metallocene molecules attached to single-walled carbon nanotubes via nickel adatoms. *Journal of Chemical Physics*, **2011**, 134, 244704 | 3.9 | 14 |
| 127 | Chapter 7:Electron Transport Theory for Large Systems. *RSC Theoretical and Computational Chemistry Series*, **2011**, 179-224 | 1.2 | 2 |
| 126 | Magnetic interaction of Co ions near the (10bar{1}0 ) ZnO surface. *New Journal of Physics*, **2010**, 12, 083061 | 3.9 | 4 |
| 125 | Controlled sequential dehydrogenation of single molecules by scanning tunneling microscopy. *Physical Review B*, **2010**, 82, | 3.3 | 15 |
| 124 | Conductance of a phenylene-vinylene molecular wire: Contact gap and tilt angle dependence. *Physical Review B*, **2010**, 81, | 3.3 | 9 |
| 123 | Quantum conductance of a single magnetic atom: An ab initio study. *Physical Review B*, **2010**, 82, | 3.3 | 19 |
| 122 | Low-bias conductance of single benzene molecules contacted by direct Au-C and Pt-C bonds. *Nanotechnology*, **2010**, 21, 495202 | 3.4 | 21 |
| 121 | Spin filter effect of manganese phthalocyanine contacted with single-walled carbon nanotube electrodes. *Journal of Chemical Physics*, **2010**, 132, 054703 | 3.9 | 44 |

| | | | |
|---|---|---|---|
| 120 | Electronic transport calculations for the conductance of Pt-1,4-phenylene diisocyanide-Pt molecular junctions. *Nanotechnology*, **2010**, 21, 155203 | 3.4 | 8 |
| 119 | Magnetism of wurtzite CoO nanoclusters. *Physical Review B*, **2010**, 81, | 3.3 | 15 |
| 118 | Polaronic distortion and vacancy-induced magnetism in MgO. *Physical Review B*, **2010**, 81, | 3.3 | 67 |
| 117 | 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 |
| 116 | Tuning the magneto-transport properties of nickel-cyclopentadienyl multidecker clusters by molecule-electrode coupling manipulation. *ACS Nano*, **2010**, 4, 2274-82 | 16.7 | 31 |
| 115 | Investigation of the conducting properties of a photoswitching dithienylethene molecule. *ACS Nano*, **2010**, 4, 2635-42 | 16.7 | 39 |
| 114 | Electronic transport across S9 sulfur clusters. *Physical Review B*, **2010**, 82, | 3.3 | 10 |
| 113 | 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 |
| 112 | Electric field response of strongly correlated one-dimensional metals: A Bethe ansatz density functional theory study. *Physical Review B*, **2010**, 82, | 3.3 | 18 |
| 111 | Spin transport properties of 3d transition metal(II) phthalocyanines in contact with single-walled carbon nanotube electrodes. *Physical Chemistry Chemical Physics*, **2010**, 12, 10805-11 | 3.6 | 59 |
| 110 | Computational modeling of a carbon nanotube-based DNA nanosensor. *Nanotechnology*, **2010**, 21, 445501 | 3.4 | 12 |
| 109 | Anomalous I-V curve for mono-atomic carbon chains. *New Journal of Physics*, **2010**, 12, 103017 | 2.9 | 15 |
| 108 | Ab initio study of electron transport in dry poly(G)-poly(C) A-DNA strands. *Physical Review B*, **2010**, 82, | 3.3 | 28 |
| 107 | Finite-bias electronic transport of molecules in a water solution. *Physical Review B*, **2010**, 81, | 3.3 | 40 |
| 106 | Selection of single-walled carbon nanotubes according to both their diameter and chirality via nanotweezers. *Nano Research*, **2010**, 3, 296-306 | 10 | 12 |
| 105 | Oxygen defect origin of ferromagnetism in ZnCoO. *Journal of Magnetism and Magnetic Materials*, **2010**, 322, 1209-1211 | 2.8 | 10 |
| 104 | Electron transport across electrically switchable magnetic molecules. *Physical Review B*, **2009**, 80, | 3.3 | 7 |
| 103 | Resonant electronic states and I-V curves of Fe/MgO/Fe(100) tunnel junctions. *Physical Review B*, **2009**, 79, | 3.3 | 53 |

| | | | |
|---|---|---|---|
| 102 | Switching a single spin on metal surfaces by a STM Tip: Ab Initio studies. *Physical Review Letters*, **2009**, 103, 057202 | 7.4 | 52 |
| 101 | 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 |
| 100 | Simulating STM transport in alkanes from first principles. *Physical Review B*, **2009**, 79, | 3.3 | 23 |
| 99 | MgN: A possible material for spintronic applications. *Physical Review B*, **2009**, 80, | 3.3 | 28 |
| 98 | Nonequilibrium Green function study of Pd4-cluster-functionalized carbon nanotubes as hydrogen sensors. *Physical Review B*, **2009**, 79, | 3.3 | 17 |
| 97 | Effects of spin-orbit coupling on the conductance of molecules contacted with gold electrodes. *Journal of Physics Condensed Matter*, **2009**, 21, 335301 | 1.8 | 6 |
| 96 | The spin filter effect of iron-cyclopentadienyl multidecker clusters: the role of the electrode band structure and the coupling strength. *Nanotechnology*, **2009**, 20, 385401 | 3.4 | 32 |
| 95 | Electronic transport calculations for rough interfaces in Al, Cu, Ag, and Au. *Journal of Physics Condensed Matter*, **2009**, 21, 315001 | 1.8 | 5 |
| 94 | Magnetism in carbon nanoscrolls: Quasi-half-metals and half-metals in pristine hydrocarbons. *Nano Research*, **2009**, 2, 844-850 | 10 | 10 |
| 93 | A spin of their own. *Nature Materials*, **2009**, 8, 693-5 | 27 | 123 |
| 92 | Electrostatic spin crossover effect in polar magnetic molecules. *Nature Materials*, **2009**, 8, 813-7 | 27 | 134 |
| 91 | Exploring the limits of the self-consistent Born approximation for inelastic electronic transport. *Physical Review B*, **2009**, 79, | 3.3 | 26 |
| 90 | Electronic transport properties of 1,1'-ferrocene dicarboxylic acid linked to Al(111) electrodes. *ACS Nano*, **2009**, 3, 4137-43 | 16.7 | 31 |
| 89 | Electron doping and magnetic moment formation in N- and C-doped MgO. *Applied Physics Letters*, **2009**, 94, 252505 | 3.4 | 70 |
| 88 | Comment on "theoretical description of carrier mediated magnetism in cobalt doped ZnO". *Physical Review Letters*, **2009**, 102, 159701; discussion 159702 | 7.4 | 14 |
| 87 | Interface and transport properties of Fe/V/MgO/Fe and Fe/V/Fe/MgO/Fe magnetic tunneling junctions. *Physical Review B*, **2009**, 79, | 3.3 | 18 |
| 86 | Ab initio calculation of the bias-dependent transport properties of Mn12 molecules. *Physical Review B*, **2009**, 80, | 3.3 | 58 |
| 85 | Effects induced by single and multiple dopants on the transport properties in zigzag-edged graphene nanoribbons. *Physical Review B*, **2009**, 80, | 3.3 | 73 |

| | | | |
|---|---|---|---|
| 84 | Magnetism of CoO polymorphs: Density functional theory and Monte Carlo simulations. *Physical Review B*, **2008**, 78, | 3.3 | 33 |
| 83 | Impurity-ion pair induced high-temperature ferromagnetism in Co-doped ZnO. *Physical Review B*, **2008**, 78, | 3.3 | 144 |
| 82 | 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 |
| 81 | IV curves of Fe/MgO (001) single- and double-barrier tunnel junctions. *Physical Review B*, **2008**, 78, | 3.3 | 19 |
| 80 | Novel one-dimensional organometallic half metals: vanadium-cyclopentadienyl, vanadium-cyclopentadienyl-benzene, and vanadium-anthracene wires. *Nano Letters*, **2008**, 8, 3640-4 | 11.5 | 116 |
| 79 | The difference of the transport properties of graphene with corrugation structure and with flat structure. *Applied Physics Letters*, **2008**, 92, 163104 | 3.4 | 11 |
| 78 | Polarizability of molecular chains: A self-interaction correction approach. *Physical Review B*, **2008**, 77, | 3.3 | 53 |
| 77 | Electronic properties of bulk and thin film SrRuO3: Search for the metal-insulator transition. *Physical Review B*, **2008**, 78, | 3.3 | 124 |
| 76 | Functionalized Nanopore-Embedded Electrodes for Rapid DNA Sequencing. *Journal of Physical Chemistry C*, **2008**, 112, 3456-3459 | 3.8 | 65 |
| 75 | Conceptual molecular quantum phase transistor based on first-principles quantum transport calculations. *Physical Review B*, **2008**, 78, | 3.3 | 24 |
| 74 | Energy alignment induced negative differential resistance: the role of hybrid states in aromatic molecular devices. *Journal of Chemical Physics*, **2008**, 129, 074710 | 3.9 | 15 |
| 73 | Efficient ab initio method for inelastic transport in nanoscale devices: Analysis of inelastic electron tunneling spectroscopy. *Physical Review B*, **2008**, 78, | 3.3 | 39 |
| 72 | Predicting d0 magnetism: Self-interaction correction scheme. *Physical Review B*, **2008**, 78, | 3.3 | 113 |
| 71 | Newtonian origin of the spin motive force in ferromagnetic atomic wires. *Physical Review B*, **2008**, 77, | 3.3 | 22 |
| 70 | Effects of self-interaction corrections on the transport properties of phenyl-based molecular junctions. *Physical Review B*, **2008**, 77, | 3.3 | 114 |
| 69 | High transmission in ruthenium–benzene–ruthenium molecular junctions. *Chemical Physics*, **2008**, 354, 106-111 | 2.3 | 17 |
| 68 | Efficient atomic self-interaction correction scheme for nonequilibrium quantum transport. *Physical Review Letters*, **2007**, 99, 056801 | 7.4 | 120 |
| 67 | 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 | 3.9 | 47 |

| | | | |
|---|---|---|---|
| 66 | Injecting and controlling spins in organic materials. *Journal of Materials Chemistry*, **2007**, 17, 4455 | | 75 |
| 65 | 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 | 24 | 41 |
| 64 | Organic electronics: memoirs of a spin. *Nature Nanotechnology*, **2007**, 2, 204-6 | 28.7 | 33 |
| 63 | Investigation of n-type donor defects in Co-doped ZnO. *Journal of Magnetism and Magnetic Materials*, **2007**, 316, e185-e187 | 2.8 | 8 |
| 62 | Magnetic properties of ZrO2-diluted magnetic semiconductors. *Journal of Magnetism and Magnetic Materials*, **2007**, 316, e188-e190 | 2.8 | 24 |
| 61 | Electronic transport through Fe/MgO/Fe(1 0 0) tunnel junctions. *Journal of Magnetism and Magnetic Materials*, **2007**, 316, 481-483 | 2.8 | 13 |
| 60 | Structure-related effects on the domain wall migration in atomic point contacts. *Journal of Magnetism and Magnetic Materials*, **2007**, 316, e934-e936 | 2.8 | |
| 59 | Monte Carlo simulations of donor band exchange in (Zn,Co)O. *Journal of Magnetism and Magnetic Materials*, **2007**, 316, 218-220 | 2.8 | 3 |
| 58 | Exchange parameters from approximate self-interaction correction scheme. *Journal of Chemical Physics*, **2007**, 127, 034112 | 3.9 | 9 |
| 57 | Effect of the continuity of the pi conjugation on the conductance of ruthenium-octene-ruthenium molecular junctions. *Journal of Chemical Physics*, **2007**, 126, 174706 | 3.9 | 9 |
| 56 | First-principles calculation on the zero-bias conductance of a gold/1,4-diaminobenzene/gold molecular junction. *Nanotechnology*, **2007**, 18, 345203 | 3.4 | 25 |
| 55 | Resonant magnetoresistance in organic spin valves (invited). *Journal of Applied Physics*, **2007**, 101, 09B102 | 2.5 | 17 |
| 54 | Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids. *Physical Review B*, **2007**, 75, | 3.3 | 139 |
| 53 | Search for magnetoresistance in excess of 1000% in Ni point contacts: Density functional calculations. *Physical Review B*, **2007**, 76, | 3.3 | 22 |
| 52 | On-site approximation for spin–orbit coupling in linear combination of atomic orbitals density functional methods. *Journal of Physics Condensed Matter*, **2007**, 19, 489001 | 1.8 | 4 |
| 51 | Giant magnetoresistance of nickel-contacted carbon nanotubes. *Journal of Physics Condensed Matter*, **2007**, 19, 042201 | 1.8 | 6 |
| 50 | First Principles Study of the Phase Transitions of MnAs. *Materials Research Society Symposia Proceedings*, **2006**, 941, 1 | | |
| 49 | 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 |

| | | | |
|---|---|---|---|
| 48 | Magnetization of electrodeposited nickel: Role of interstitial carbon. *Journal of Applied Physics*, **2006**, 99, 08J301 | 2.5 | 6 |
| 47 | Inelastic transport in molecular spin valves: Calculations using the tight-binding Su-Schrieffer-Heeger model. *Physical Review B*, **2006**, 73, | 3.3 | 10 |
| 46 | Magnetomechanical interplay in spin-polarized point contacts. *Physical Review B*, **2006**, 73, | 3.3 | 2 |
| 45 | Bias Dependent TMR in Fe/MgO/Fe(100) Tunnel Junctions. *Materials Research Society Symposia Proceedings*, **2006**, 941, 1 | | |
| 44 | Ab initio study of the magnetostructural properties of MnAs. *Physical Review B*, **2006**, 74, | 3.3 | 39 |
| 43 | Spin and molecular electronics in atomically generated orbital landscapes. *Physical Review B*, **2006**, 73, | 3.3 | 551 |
| 42 | Molecular conduction: do time-dependent simulations tell you more than the Landauer approach?. *Journal of Chemical Physics*, **2006**, 124, 214708 | 3.9 | 67 |
| 41 | Molecular-Spintronics: The Art of Driving Spin Through Molecules. *Journal of Computational and Theoretical Nanoscience*, **2006**, 3, 624-642 | 0.3 | 123 |
| 40 | Molecular-Spintronics: The Art of Driving Spin Through Molecules. *Journal of Computational and Theoretical Nanoscience*, **2006**, 3, 624-642 | 0.3 | 89 |
| 39 | Ferromagnetism driven by intrinsic point defects in HfO(2). *Physical Review Letters*, **2005**, 94, 217205 | 7.4 | 383 |
| 38 | Lattice distortion effects on the magnetostructural phase transition of MnAs. *Physical Review Letters*, **2005**, 95, 077203 | 7.4 | 22 |
| 37 | Self-interaction errors in density-functional calculations of electronic transport. *Physical Review Letters*, **2005**, 95, 146402 | 7.4 | 277 |
| 36 | Strong correlation and ferromagnetism in (Ga,Mn)As and (Ga,Mn)N. *Journal of Magnetism and Magnetic Materials*, **2005**, 290-291, 1391-1394 | 2.8 | 11 |
| 35 | Self-interaction effects in (Ga,Mn)As and (Ga,Mn)N. *Chemical Physics*, **2005**, 309, 59-65 | 2.3 | 36 |
| 34 | Towards molecular spintronics. *Nature Materials*, **2005**, 4, 335-9 | 27 | 1096 |
| 33 | Magnetic proximity effect in carbon nanotubes. *Journal of Magnetism and Magnetic Materials*, **2005**, 290-291, 286-289 | 2.8 | 4 |
| 32 | Current-driven magnetic rearrangements in spin-polarized point contacts. *Physical Review B*, **2005**, 72, | 3.3 | 19 |
| 31 | Single-channel conductance of H2 molecules attached to platinum or palladium electrodes. *Physical Review B*, **2005**, 72, | 3.3 | 41 |

| | | | |
|---|---|---|---|
| 30 | Conductance oscillations in zigzag platinum chains. *Physical Review Letters*, **2005**, 95, 256804 | 7.4 | 50 |
| 29 | Asymmetric I-V characteristics and magnetoresistance in magnetic point contacts. *Physical Review B*, **2004**, 70, | 3.3 | 45 |
| 28 | Contact-induced spin polarization in carbon nanotubes. *Physical Review B*, **2004**, 69, | 3.3 | 24 |
| 27 | The magnetism of carbon. *Physics World*, **2004**, 17, 33-37 | 0.5 | 14 |
| 26 | Magnetic semiconductors and half-metals. *Journal Physics D: Applied Physics*, **2004**, 37, 988-993 | 3 | 123 |
| 25 | I-V asymmetry and magnetoresistance in nickel nanoconstrictions. *Journal of Magnetism and Magnetic Materials*, **2004**, 272-276, 1571-1572 | 2.8 | 9 |
| 24 | (Ga,Mn)As/AlAs digital ferromagnetic heterostructures. *Journal of Magnetism and Magnetic Materials*, **2004**, 272-276, E1583-E1584 | 2.8 | |
| 23 | Contact induced magnetism in carbon nanotubes. *Journal of Physics Condensed Matter*, **2004**, 16, L155-L161 | 1.8 | 80 |
| 22 | Different origins of the ferromagnetic order in (Ga,Mn)As and (Ga,Mn)N. *Physical Review B*, **2004**, 70, | 3.3 | 111 |
| 21 | Ferromagnetism and metallic state in digital (Ga,Mn)As heterostructures. *Physical Review B*, **2003**, 68, | 3.3 | 20 |
| 20 | Quantum Transport in Inhomogeneous Multi-Wall Nanotubes **2002**, 333-347 | | |
| 19 | Prediction of enhanced ferromagnetism in (Ga,Mn)As by intrinsic defect manipulation. *Journal of Magnetism and Magnetic Materials*, **2002**, 238, 252-257 | 2.8 | 5 |
| 18 | First principles study of intrinsic defects in (Ga,Mn)As. *Journal of Magnetism and Magnetic Materials*, **2002**, 242-245, 441-446 | 2.8 | 9 |
| 17 | Density Functional Calculations for III-V Diluted Ferromagnetic Semiconductors: A Review. *Journal of Superconductivity and Novel Magnetism*, **2002**, 15, 85-104 | | 78 |
| 16 | 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 |
| 15 | Spin-Polarized Transport in F/S Nanojunctions. *Journal of Low Temperature Physics*, **2001**, 124, 305-320 | 1.3 | 8 |
| 14 | Ab initio transport theory for digital ferromagnetic heterostructures. *Physical Review Letters*, **2001**, 87, 267202 | 7.4 | 42 |
| 13 | Influence of the local As antisite distribution on ferromagnetism in (Ga, Mn)As. *Applied Physics Letters*, **2001**, 78, 3493-3495 | 3.4 | 65 |

| | | | |
|---|---|---|---|
| 12 | First-principles study of the origin and nature of ferromagnetism in Ga1−xMnxAs. *Physical Review B*, **2001**, 63, | 3.3 | 258 |
| 11 | Anomalous magnetoresistance of magnetic multilayers. *Journal of Physics Condensed Matter*, **2000**, 12, L621-L626 | 1.8 | |
| 10 | Breakdown of the resistor model of CPP-GMR in magnetic multilayered nanostructures. *Physical Review B*, **2000**, 61, 14225-14228 | 3.3 | 12 |
| 9 | Enhancement of giant magnetoresistance due to spin mixing in magnetic multilayers with a superconducting contact. *Physical Review B*, **2000**, 63, | 3.3 | 6 |
| 8 | Fractional quantum conductance in carbon nanotubes. *Physical Review Letters*, **2000**, 84, 1974-7 | 7.4 | 150 |
| 7 | Ground state of half-metallic zinc-blende MnAs. *Physical Review B*, **2000**, 62, 15553-15560 | 3.3 | 211 |
| 6 | Suppression of Giant Magnetoresistance by a Superconducting Contact. *Physical Review Letters*, **1999**, 82, 4938-4941 | 7.4 | 20 |
| 5 | Crossover between the ballistic and diffusive regime of the spin-conductance and giant magnetoresistance in magnetic multilayered nanostructures. *Physical Review B*, **1999**, 60, 7385-7394 | 3.3 | 12 |
| 4 | GMR in 3d, 4d and 5d transition metals multilayers. *Journal of Magnetism and Magnetic Materials*, **1999**, 196-197, 101-103 | 2.8 | 3 |
| 3 | 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 |
| 2 | A further look at waveguide lasers. *IEEE Journal of Quantum Electronics*, **1998**, 34, 2403-2408 | 2 | 0 |
| 1 | Conductance oscillations in transition metal superlattices. *Journal of Physics Condensed Matter*, **1998**, 10, L691-L697 | 1.8 | 4 |