Federico Totti

List of Publications by Year in Descending Order

97 papers	3,519 citations	30 h-index	56 g-index
100 ext. papers	4,017 ext. citations	7.5 avg, IF	5.25 L-index

#	Paper	IF	Citations
97	Innovative Characterization of Original Green Vanillin-derived Schiff Bases as Corrosion Inhibitors by A Synergic Approach Based on Electrochemistry, Microstructure, and Computational Analyses. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2022**, 641, 128540	5.1	2
96	Engineering Chemisorption of Fe4 Single-Molecule Magnets on Gold. *Advanced Materials Interfaces*, **2021**, 8, 2101182	4.6	1
95	Magnetic Anisotropy Trends along a Full 4f-Series: The Effect. *Journal of the American Chemical Society*, **2021**, 143, 8108-8115	16.4	15
94	Exploring the Organometallic Route to Molecular Spin Qubits: The [CpTi(cot)] Case. *Angewandte Chemie*, **2021**, 133, 2620-2625	3.6	8
93	Exploring the Organometallic Route to Molecular Spin Qubits: The [CpTi(cot)] Case. *Angewandte Chemie - International Edition*, **2021**, 60, 2588-2593	16.4	14
92	Probing Vibrational Symmetry Effects and Nuclear Spin Economy Principles in Molecular Spin Qubits. *Inorganic Chemistry*, **2021**, 60, 140-151	5.1	11
91	Magnetic anisotropy on demand exploiting high-pressure as remote control: an proof of concept. *Dalton Transactions*, **2021**, 50, 10621-10628	4.3	2
90	A Complete View of Orbach and Raman Spin-Lattice Relaxation in a Dysprosium Coordination Compound. *Journal of the American Chemical Society*, **2021**, 143, 13633-13645	16.4	26
89	Temperature Dependence of Spin-Phonon Coupling in [VO(acac)]: A Computational and Spectroscopic Study. *Journal of Physical Chemistry C*, **2021**, 125, 22100-22110	3.8	5
88	Chemisorption of nitronyl-nitroxide radicals on gold surface: an assessment of morphology, exchange interaction and decoherence time. *Nanoscale*, **2021**, 13, 7613-7621	7.7	4
87	Hetero-tri-spin systems: an alternative stairway to the single molecule magnet heaven?. *Dalton Transactions*, **2021**, 50, 15961-15972	4.3	1
86	Quantum dynamics of a single molecule magnet on superconducting Pb(111). *Nature Materials*, **2020**, 19, 546-551	27	24
85	The Origin of Magnetic Anisotropy and Single-Molecule Magnet Behavior in Chromium(II)-Based Extended Metal Atom Chains. *Inorganic Chemistry*, **2020**, 59, 1763-1777	5.1	12
84	An Oxalate-Bridged Copper(II) Complex Combining Monodentate Benzoate, 2,2′-bipyridine and Aqua Ligands: Synthesis, Crystal Structure and Investigation of Magnetic Properties. *Molecules*, **2020**, 25,	4.8	5
83	Quantitative and Chemically Intuitive Evaluation of the Nature of M-L Bonds in Paramagnetic Compounds: Application of EDA-NOCV Theory to Spin Crossover Complexes. *Chemistry - A European Journal*, **2020**, 26, 13677-13685	4.8	5
82	Study of three new halogenated oxoquinolinecarbohydrazide N-phosphonate derivatives as corrosion inhibitor for mild steel in acid environment. *Surfaces and Interfaces*, **2020**, 21, 100773	4.1	7
81	SMM Behavior Tuned by an Exchange Coupling LEGO Approach for Chimeric Compounds: First 2p-3d-4f Heterotrispin Complexes with Different Metal Ions Bridged by One Aminoxyl Group. *Inorganic Chemistry*, **2019**, 58, 13090-13101	5.1	30

80	Vanadyl phthalocyanines on graphene/SiC(0001): toward a hybrid architecture for molecular spin qubits. *Nanoscale Horizons*, **2019**, 4, 1202-1210	10.8	17
79	Covalency and magnetic anisotropy in lanthanide single molecule magnets: the DyDOTA archetype. *Chemical Science*, **2019**, 10, 7233-7245	9.4	35
78	Redox-Active Dysprosium Single-Molecule Magnet: Spectro-Electrochemistry and Theoretical Investigations. *Magnetochemistry*, **2019**, 5, 46	3.1	2
77	Surface effects on a photochromic spin-crossover iron(ii) molecular switch adsorbed on highly oriented pyrolytic graphite. *Nanoscale*, **2019**, 11, 20006-20014	7.7	13
76	Magnetic Cationic Copper(II) Chains and a Mononuclear Cobalt(II) Complex Containing [Ln(hfac)] Blocks as Counterions. *Inorganic Chemistry*, **2019**, 58, 1976-1987	5.1	14
75	Tetrathiafulvalene-Based Helicene Ligand in the Design of a Dysprosium Field-Induced Single-Molecule Magnet. *Inorganic Chemistry*, **2019**, 58, 52-56	5.1	22
74	Mössbauer spectroscopy of a monolayer of single molecule magnets. *Nature Communications*, **2018**, 9, 480	17.4	25
73	The disclosure of mesoscale behaviour of a 3d-SMM monolayer on Au(111) through a multilevel approach. *Nanoscale*, **2018**, 10, 4096-4104	7.7	4
72	Magnetic Slow Relaxation in a Metal-Organic Framework Made of Chains of Ferromagnetically Coupled Single-Molecule Magnets. *Chemistry - A European Journal*, **2018**, 24, 6983-6991	4.8	54
71	Room temperature control of spin states in a thin film of a photochromic iron(II) complex. *Materials Horizons*, **2018**, 5, 506-513	14.4	30
70	Solution structure of a pentachromium(ii) single molecule magnet from DFT calculations, isotopic labelling and multinuclear NMR spectroscopy. *Dalton Transactions*, **2018**, 47, 585-595	4.3	6
69	A Dy Cubane: A New Member in the Single-Molecule Toroics Family. *Angewandte Chemie - International Edition*, **2018**, 57, 17089-17093	16.4	29
68	A Dy4 Cubane: A New Member in the Single-Molecule Toroics Family. *Angewandte Chemie*, **2018**, 130, 17335-17339	3.6	4
67	Tunable Spin-Superconductor Coupling of Spin 1/2 Vanadyl Phthalocyanine Molecules. *Nano Letters*, **2018**, 18, 7955-7961	11.5	36
66	Lanthanide complexes involving multichelating TTF-based ligands. *Inorganic Chemistry Frontiers*, **2017**, 4, 604-617	6.8	18
65	A chimeric design of heterospin 2p-3d, 2p-4f, and 2p-3d-4f complexes using a novel family of paramagnetic dissymmetric compartmental ligands. *Chemical Communications*, **2017**, 53, 6504-6507	5.8	40
64	Intra-molecular origin of the spin-phonon coupling in slow-relaxing molecular magnets. *Chemical Science*, **2017**, 8, 6051-6059	9.4	112
63	Slow Magnetic Relaxation in Chiral Helicene-Based Coordination Complex of Dysprosium. *Magnetochemistry*, **2017**, 3, 2	3.1	13

62	The role of anharmonic phonons in under-barrier spin relaxation of single molecule magnets. *Nature Communications*, **2017**, 8, 14620	17.4	215
61	Di- and Triphosphate Recognition and Sensing with Mono- and Dinuclear Fluorescent Zinc(II) Complexes: Clues for the Design of Selective Chemosensors for Anions in Aqueous Media. *Chemistry - A European Journal*, **2016**, 22, 14890-14901	4.8	13
60	Improved slow magnetic relaxation in optically pure helicene-based Dy single molecule magnets. *Chemical Communications*, **2016**, 52, 14474-14477	5.8	41
59	Giant spin-phonon bottleneck effects in evaporable vanadyl-based molecules with long spin coherence. *Dalton Transactions*, **2016**, 45, 16635-16643	4.3	61
58	Binuclear Lanthanide-Radical Complexes Featuring Two Centers with Different Magnetic and Luminescence Properties. *Inorganic Chemistry*, **2016**, 55, 11676-11684	5.1	25
57	Relaxation Dynamics and Magnetic Anisotropy in a Low-Symmetry Dy(III) Complex. *Chemistry - A European Journal*, **2016**, 22, 5552-62	4.8	52
56	Toward Mesoscale Properties of Self-Assembled Monolayers of SMM on Au(111): An Integrated Ad Hoc FF and DFT Study. *Journal of Physical Chemistry C*, **2016**, 120, 14774-14781	3.8	4
55	First coordination compounds based on a bis(imino nitroxide) biradical and 4f metal ions: synthesis, crystal structures and magnetic properties. *Dalton Transactions*, **2016**, 45, 2936-44	4.3	27
54	The Role of Anisotropic Exchange in Single Molecule Magnets: A CASSCF/NEVPT2 Study of the Fe4 SMM Building Block [Fe2(OCH3)2(dbm)4] Dimer. *Inorganics*, **2016**, 4, 28	2.9	12
53	Highly Axial Magnetic Anisotropy in a N O Dysprosium(III) Coordination Environment Generated by a Merocyanine Ligand. *Chemistry - A European Journal*, **2016**, 22, 15222-15226	4.8	13
52	The Challenge of Thermal Deposition of Coordination Compounds: Insight into the Case of an Fe4 Single Molecule Magnet. *Chemistry of Materials*, **2016**, 28, 7693-7702	9.6	10
51	cis-Pt I2(NH3)2: a reappraisal. *Dalton Transactions*, **2015**, 44, 14896-905	4.3	40
50	Single molecule magnets grafted on gold: magnetic properties from ab initio molecular dynamics. *Journal of Materials Chemistry C*, **2015**, 3, 7294-7304	7.1	16
49	Magnetic bistability in a submonolayer of sublimated Fe4 single-molecule magnets. *Nano Letters*, **2015**, 15, 535-41	11.5	57
48	Magnetic fingerprint of individual Fe4 molecular magnets under compression by a scanning tunnelling microscope. *Nature Communications*, **2015**, 6, 8216	17.4	46
47	Molecular magnets and surfaces: A promising marriage. A DFT insight. *Coordination Chemistry Reviews*, **2015**, 289-290, 357-378	23.2	46
46	DFT magnetic characterization of a Fe4 SMMs series: from isotropic exchange interactions to multi-spin zero field splitting. *Journal of Materials Chemistry C*, **2014**, 2, 8333-8343	7.1	13
45	A Combined Ion Scattering, Photoemission, and DFT Investigation on the Termination Layer of a La0.7Sr0.3MnO3 Spin Injecting Electrode. *Journal of Physical Chemistry C*, **2014**, 118, 13631-13637	3.8	22

44	UHV deposition and characterization of a mononuclear iron(III) □diketonate complex on Au(111). *Beilstein Journal of Nanotechnology*, **2014**, 5, 2139-48	3	6
43	Valence electronic structure of sublimated Fe4 single-molecule magnets: an experimental and theoretical characterization. *Journal of Materials Chemistry C*, **2014**, 2, 9599-9608	7.1	21
42	Dynamic control of magnetic nanowires by light-induced domain-wall kickoffs. *Nature Materials*, **2013**, 12, 202-6	27	42
41	Enhanced vapor-phase processing in fluorinated Fe4 single-molecule magnets. *Inorganic Chemistry*, **2013**, 52, 5897-905	5.1	24
40	Computational Studies on SAMs of {Mn6} SMMs on Au(111): Do Properties Change upon Grafting?. *Journal of Physical Chemistry C*, **2013**, 117, 7186-7190	3.8	13
39	On the kinetics and thermodynamics of S□X (X = H, CH3, SCH3, COCH3, and CN) cleavage in the formation of self-assembled monolayers of alkylthiols on Au(111). *Highlights in Theoretical Chemistry*, **2013**, 99-109		
38	On the kinetics and thermodynamics of S□X (X = H, CH3, SCH3, COCH3, and CN) cleavage in the formation of self-assembled monolayers of alkylthiols on Au(111). *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	15
37	A periodic mixed gaussians-plane waves DFT study on simple thiols on Au(111): adsorbate species, surface reconstruction, and thiols functionalization. *Physical Chemistry Chemical Physics*, **2011**, 13, 3886-95	3.6	29
36	Synthesis and characterization of new oligomeric and polymeric complexes based on the [CuII(bpca)]+ unit [Hbpca = bis(2-pyridylcarbonyl)amine]. *Inorganica Chimica Acta*, **2011**, 376, 538-548	2.7	13
35	Quantum tunnelling of the magnetization in a monolayer of oriented single-molecule magnets. *Nature*, **2010**, 468, 417-21	50.4	515
34	A DFT exploration of the organization of thiols on Au(111): a route to self-assembled monolayer of magnetic molecules. *Journal of Materials Chemistry*, **2010**, 20, 10747		20
33	Polyamine receptors containing dipyridine or phenanthroline units: clues for the design of fluorescent chemosensors for metal ions. *Chemistry - A European Journal*, **2009**, 15, 8049-63	4.8	25
32	Modeling thiols on Au(111): Structural, thermodynamic and magnetic properties of simple thiols and thiol-radicals. *Superlattices and Microstructures*, **2009**, 46, 4-9	2.8	17
31	Density functional studies on the exchange interaction of a dinuclear Gd(iii)-Cu(ii) complex: method assessment, magnetic coupling mechanism and magneto-structural correlations. *Dalton Transactions*, **2009**, 3153-61	4.3	129
30	A Few Comments on the Application of Density Functional Theory to the Calculation of the Magnetic Structure of Oligo-Nuclear Transition Metal Clusters. *Journal of Chemical Theory and Computation*, **2009**, 5, 144-54	6.4	88
29	On the importance of the biquadratic terms in exchange coupled systems: A post-HF investigation. *Inorganica Chimica Acta*, **2008**, 361, 4153-4156	2.7	17
28	Magnetic and optical properties of Cu(II)-bis(oxamato) complexes: combined quantum chemical density functional theory and vibrational spectroscopy studies. *Journal of Physical Chemistry B*, **2008**, 112, 5585-93	3.4	10
27	Mononuclear, dinuclear, and pentanuclear [[N,S(thiolate)]iron(II)] complexes: nuclearity control, incorporation of hydroxide bridging ligands, and magnetic behavior. *Chemistry - A European Journal*, **2005**, 11, 7328-41	4.8	24

26	DFT description of the magnetic structure of polynuclear transition-metal clusters: The complexes [{Cu(bpca)2(H2O)2}{Cu(NO3)2}2], (bpca = Bis(2-pyridylcarbonyl)amine), and [Cu(DBSQ)(C2H5O)]2, (DBSQ = 3,5-di-tert-butyl-semiquinonato). *International Journal of Quantum Chemistry*, **2005**, 101, 819-825	2.1	60
25	Strong ferromagnetic interactions in [V(8)O(14)(H(_2)taci)(2)]: an unprecedented large spin ground state for a vanadyl cluster. *Angewandte Chemie - International Edition*, **2004**, 43, 3436-9	16.4	74
24	Strong Ferromagnetic Interactions in [V8O14(H2taci)2]: An Unprecedented Large Spin Ground State for a Vanadyl Cluster. *Angewandte Chemie*, **2004**, 116, 3518-3521	3.6	13
23	DFT description of the electronic structure and spectromagnetic properties of strongly correlated electronic systems: NiII, CuII and ZnII o-dioxolene complexes. *Chemistry - A European Journal*, **2004**, 10, 1472-80	4.8	11
22	A dinuclear copper(II) complex with a Cu(O, NO)Cu bridging core: structural and magnetic (experimental and density functional theory) studies. *Inorganica Chimica Acta*, **2004**, 357, 2150-2156	2.7	12
21	Density functional characterization of the chemoselective oxidation of catechol by using molecular oxygen: thermodynamics of the reaction between [(triphos)Ir(dtbc)]+ and O2. *Chemistry - A European Journal*, **2003**, 9, 3015-23	4.8	6
20	Crystal and molecular structure and magnetic exchange properties of bis(di-micro-ethoxo-bis(3,5-di-tert-butylsemiquinonato)dicopper(II)) complex. A synergy between DFT and experimental magnetochemistry. *Inorganic Chemistry*, **2003**, 42, 8065-71	5.1	28
19	Mono- and di-nuclear tris(pyrazolyl)borato-oxo-tungsten(V) complexes with phenolate ligands: syntheses and structures, and magnetic, electrochemical and UV/Vis/NIR spectroscopic properties. *Dalton Transactions*, **2003**, 36-45	4.3	21
18	DFT description of the magnetic properties and electron localization in dinuclear di-mu-oxo-bridged manganese complexes. *Chemistry - A European Journal*, **2002**, 8, 5019-27	4.8	31
17	Electronic and magnetic metal metal interactions in dinuclear oxomolybdenum(V) complexes across bis-phenolate bridging ligands with different spacers between the phenolate termini: ligand-centred vs. metal-centred redox activity. *Dalton Transactions RSC*, **2001**, 1401-1414		36
16	Spin-Density Map of the Triplet Ground State of a Titanium(IV) Complex with Schiff-Base Diquinone Radical Ligands: An Investigation Using Polarized-Neutron Diffraction and Density-Functional Theory This work was supported by the 3MD EU network (contract ERB 4061 PL 97-0197). *Angewandte Chemie - International Edition*, **2000**, 39, 1786-1788	16.4	17
15	Density functional description of the early stages of the dioxygenation of [(MeC(CH2PPh2)3)M(catecholate)]+ complexes [M = Co(III), Ir(III)]: toward a rationalization of the catalytic mechanism of ring-opening dioxygenases. *Inorganic Chemistry*, **2000**, 39, 1418-25	5.1	8
14	Metal-metal interactions as a function of bridging ligand topology: an electrochemical, spectroelectrochemical, and magnetic study on dinuclear Oxo-Mo(V) complexes with various isomers of dihydroxynaphthalene as bridging ligand. *Inorganic Chemistry*, **2000**, 39, 1288-93	5.1	27
13	On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems: The Case of the Ferromagnetic Copper(II) &mgr;(2)-Azido Bridged Complexes. *Inorganic Chemistry*, **1999**, 38, 1996-2004	5.1	154
12	Tetranuclear grid-like copper(II) complexes with pyrazolate bridges: syntheses, structures, magnetic and EPR spectroscopic properties. *Journal of the Chemical Society Dalton Transactions*, **1999**, 339-348		63
11	DFT Description of Mixed Valence Magnetic Systems. Mn(III)-Mn(IV) and Fe(II)-Fe(III) Complexes. *Molecular Crystals and Liquid Crystals*, **1999**, 335, 665-674		4
10	Electrochemical and Magnetic Exchange Interactions in Trinuclear Chain Complexes Containing Oxo-Mo(V) Fragments as a Function of the Topology of the Bridging Ligand. *Inorganic Chemistry*, **1999**, 38, 365-369	5.1	41
9	Density Functional Modeling of Double Exchange Interactions in Transition Metal Complexes. Calculation of the Ground and Excited State Properties of [Fe2(OH)3(tmtacn)2]2+. *Journal of the American Chemical Society*, **1998**, 120, 8357-8365	16.4	45

8	Assessment of a Combined QM/MM Approach for the Study of Large Nitroxide Systems in Vacuo and in Condensed Phases. *Journal of the American Chemical Society*, **1998**, 120, 7069-7078	16.4	94
7	Density Functional Modeling of Long Range Magnetic Interactions in Binuclear Oxomolybdenum(V) Complexes. *Journal of Physical Chemistry A*, **1998**, 102, 10545-10551	2.8	65
6	Density Functional Calculations of Magnetic Exchange Interactions in Polynuclear Transition Metal Complexes. *Inorganic Chemistry*, **1997**, 36, 5022-5030	5.1	203
5	Roles of Bridging Ligand Topology and Conformation in Controlling Exchange Interactions between Paramagnetic Molybdenum Fragments in Dinuclear and Trinuclear Complexes. *Inorganic Chemistry*, **1997**, 36, 3447-3454	5.1	85
4	Comparison between post-Hartree-Fock and DFT methods for the study of strength and mechanism of cleavage of Hg(SINGLE BOND)C bond. *International Journal of Quantum Chemistry*, **1997**, 61, 361-367	2.1	13
3	Theoretical Characterization of the Mechanism of Hg□ Bond Cleavage by Halogenic Acids. *Organometallics*, **1996**, 15, 1465-1469	3.8	20
2	Theoretical Study of the Electronic Structure and of the Mercury-Carbon Bonding of Methylmercury(II) Compounds. *The Journal of Physical Chemistry*, **1995**, 99, 12743-12750		17
1	Accurate prediction of pressure and temperature T1/2 variation in solid state spin crossover by ab initio methods: the [CoII(dpzca)2] case. *Journal of Materials Chemistry C*,	7.1	2