Federico Totti

List of Publications by Year in descending order

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97 papers	4,535 citations	117453 34 h-index	110170 64 g-index
100 all docs	100 docs citations	100 times ranked	4103 citing authors

#	Article	IF	Citations
1	Quantum tunnelling of the magnetization in a monolayer of oriented single-molecule magnets. Nature, 2010, 468, 417-421.	13.7	574
2	The role of anharmonic phonons in under-barrier spin relaxation of single molecule magnets. Nature Communications, 2017, 8, 14620.	5.8	319
3	Density Functional Calculations of Magnetic Exchange Interactions in Polynuclear Transition Metal Complexes. Inorganic Chemistry, 1997, 36, 5022-5030.	1.9	226
4	On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems:Â The Case of the Ferromagnetic Copper(II) Î¼-Azido Bridged Complexes. Inorganic Chemistry, 1999, 38, 1996-2004.	1.9	173
5	Intra-molecular origin of the spin-phonon coupling in slow-relaxing molecular magnets. Chemical Science, 2017, 8, 6051-6059.	3.7	160
6	Density functional studies on the exchange interaction of a dinuclear Gd(iii)â€“Cu(ii) complex: method assessment, magnetic coupling mechanism and magneto-structural correlations. Dalton Transactions, 2009, , 3153.	1.6	145
7	A Complete Ab Initio View of Orbach and Raman Spinâ€“Lattice Relaxation in a Dysprosium Coordination Compound. Journal of the American Chemical Society, 2021, 143, 13633-13645.	6.6	116
8	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, 144-154.	2.3	104
9	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.	6.6	100
10	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.	1.9	99
11	Strong Ferromagnetic Interactions in [V8O14(Hâ€2taci)2]: An Unprecedented Large Spin Ground State for a Vanadyl Cluster. Angewandte Chemie - International Edition, 2004, 43, 3436-3439.	7.2	77
12	Giant spinâ€“phonon bottleneck effects in evaporable vanadyl-based molecules with long spin coherence. Dalton Transactions, 2016, 45, 16635-16643.	1.6	75
13	Density Functional Modeling of Long Range Magnetic Interactions in Binuclear Oxomolybdenum(V) Complexes. Journal of Physical Chemistry A, 1998, 102, 10545-10551.	1.1	72
14	Tunable Spinâ€“Superconductor Coupling of Spin 1/2 Vanadyl Phthalocyanine Molecules. Nano Letters, 2018, 18, 7955-7961.	4.5	72
15	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.	1.1	65
16	Magnetic Slow Relaxation in a Metalâ€“Organic Framework Made of Chains of Ferromagnetically Coupled Singleâ€Molecule Magnets. Chemistry - A European Journal, 2018, 24, 6983-6991.	1.7	64
17	Covalency and magnetic anisotropy in lanthanide single molecule magnets: the DyDOTA archetype. Chemical Science, 2019, 10, 7233-7245.	3.7	64
18	Magnetic Bistability in a Submonolayer of Sublimated Fe₄ Single-Molecule Magnets. Nano Letters, 2015, 15, 535-541.	4.5	63

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19	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) Tj ET Q q 1 1 0.78	1.0	78
20	Quantum dynamics of a single molecule magnet on superconducting Pb(111). Nature Materials, 2020, 19, 546-551.	13.3	62
21	Magnetic fingerprint of individual Fe4 molecular magnets under compression by a scanning tunnelling microscope. Nature Communications, 2015, 6, 8216.	5.8	56
22	Improved slow magnetic relaxation in optically pure helicene-based Dy^{III} single molecule magnets. Chemical Communications, 2016, 52, 14474-14477.	2.2	56
23	Relaxation Dynamics and Magnetic Anisotropy in a Lowâ€Symmetry Dy^{III} Complex. Chemistry - A European Journal, 2016, 22, 5552-5562.	1.7	56
24	Molecular magnets and surfaces: A promising marriage. A DFT insight. Coordination Chemistry Reviews, 2015, 289-290, 357-378.	9.5	55
25	A chimeric design of heterospin 2pâ€“3d, 2pâ€“4f, and 2pâ€“3dâ€“4f complexes using a novel family of paramagnetic dissymmetric compartmental ligands. Chemical Communications, 2017, 53, 6504-6507.	2.2	55
26	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.	6.6	52
27	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.	1.9	52
28	SMM Behavior Tuned by an Exchange Coupling LEGO Approach for Chimeric Compounds: First 2pâ€“3dâ€“4f Heterotrispin Complexes with Different Metal Ions Bridged by One Aminoxyl Group. Inorganic Chemistry, 2019, 58, 13090-13101.	1.9	51
29	Magnetic Anisotropy Trends along a Full 4f-Series: The fⁿ⁺⁷ Effect. Journal of the American Chemical Society, 2021, 143, 8108-8115.	6.6	50
30	cis-Pt I₂(NH₃)₂: a reappraisal. Dalton Transactions, 2015, 44, 14896-14905.	1.6	45
31	Dynamic control of magnetic nanowires by light-induced domain-wall kickoffs. Nature Materials, 2013, 12, 202-206.	13.3	44
32	Room temperature control of spin states in a thin film of a photochromic iron(<scp>ii</scp>) complex. Materials Horizons, 2018, 5, 506-513.	6.4	43
33	Electronic and magnetic metalâ€“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.	2.3	38
34	A Dy₄ Cubane: A New Member in the Singleâ€Molecule Toroics Family. Angewandte Chemie - International Edition, 2018, 57, 17089-17093.	7.2	38
35	Exploring the Organometallic Route to Molecular Spin Qubits: Theâ€‰[CpTi(cot)] Case. Angewandte Chemie - International Edition, 2021, 60, 2588-2593.	7.2	38
36	MÃ¶ssbauer spectroscopy of a monolayer of single molecule magnets. Nature Communications, 2018, 9, 480.	5.8	37

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37	Probing Vibrational Symmetry Effects and Nuclear Spin Economy Principles in Molecular Spin Qubits. Inorganic Chemistry, 2021, 60, 140-151.	1.9	35
38	First coordination compounds based on a bis(imino nitroxide) biradical and 4f metal ions: synthesis, crystal structures and magnetic properties. Dalton Transactions, 2016, 45, 2936-2944.	1.6	33
39	Metalâ^'Metal Interactions as a Function of Bridging Ligand Topology:Â An Electrochemical, Spectroelectrochemical, and Magnetic Study on Dinuclear Oxo-Mo(V) Complexes with Various Isomers of Dihydroxynaphthalene as Bridging Ligand. Inorganic Chemistry, 2000, 39, 1288-1293.	1.9	32
40	A periodic mixed gaussiansâ€"plane waves DFT study on simple thiols on Au(111): adsorbate species, surface reconstruction, and thiols functionalization. Physical Chemistry Chemical Physics, 2011, 13, 3886.	1.3	32
41	Vanadyl phthalocyanines on graphene/SiC(0001): toward a hybrid architecture for molecular spin qubits. Nanoscale Horizons, 2019, 4, 1202-1210.	4.1	32
42	DFT Description of the Magnetic Properties and Electron Localization in Dinuclear Di-μ-oxo-Bridged Manganese Complexes. Chemistry - A European Journal, 2002, 8, 5019-5027.	1.7	31
43	Crystal and Molecular Structure and Magnetic Exchange Properties of Bis(di-Î¼-ethoxo-bis(3,5-di-tert-butylsemiquinonato)dicopper(II)) Complex. A Synergy between DFT and Experimental Magnetochemistry. Inorganic Chemistry, 2003, 42, 8065-8071.	1.9	31
44	Binuclear Lanthanide-Radical Complexes Featuring Two Centers with Different Magnetic and Luminescence Properties. Inorganic Chemistry, 2016, 55, 11676-11684.	1.9	30
45	Tetrathiafulvalene-Based Helicene Ligand in the Design of a Dysprosium Field-Induced Single-Molecule Magnet. Inorganic Chemistry, 2019, 58, 52-56.	1.9	30
46	The Origin of Magnetic Anisotropy and Single-Molecule Magnet Behavior in Chromium(II)-Based Extended Metal Atom Chains. Inorganic Chemistry, 2020, 59, 1763-1777.	1.9	29
47	Enhanced Vapor-Phase Processing in Fluorinated Fe₄ Single-Molecule Magnets. Inorganic Chemistry, 2013, 52, 5897-5905.	1.9	28
48	Polyamine Receptors Containing Dipyridine or Phenanthroline Units: Clues for the Design of Fluorescent Chemosensors for Metal Ions. Chemistry - A European Journal, 2009, 15, 8049-8063.	1.7	27
49	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, 7328-7341.	1.7	26
50	Valence electronic structure of sublimated Fe₄single-molecule magnets: an experimental and theoretical characterization. Journal of Materials Chemistry C, 2014, 2, 9599-9608.	2.7	25
51	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.	6.7	24
52	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.	2.3	24
53	Theoretical Characterization of the Mechanism of Hgâ^'C Bond Cleavage by Halogenic Acids. Organometallics, 1996, 15, 1465-1469.	1.1	23
54	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.	1.6	23

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55	A Combined Ion Scattering, Photoemission, and DFT Investigation on the Termination Layer of a La_{0.7}Sr_{0.3}MnO₃ Spin Injecting Electrode. Journal of Physical Chemistry C, 2014, 118, 13631-13637.	1.5	23
56	Single molecule magnets grafted on gold: magnetic properties from ab initio molecular dynamics. Journal of Materials Chemistry C, 2015, 3, 7294-7304.	2.7	22
57	Modeling thiols on Au(111): Structural, thermodynamic and magnetic properties of simple thiols and thiol-radicals. Superlattices and Microstructures, 2009, 46, 4-9.	1.4	21
58	Lanthanide complexes involving multichelating TTF-based ligands. Inorganic Chemistry Frontiers, 2017, 4, 604-617.	3.0	21
59	Exploring the Organometallic Route to Molecular Spin Qubits: Theâ€‰[CpTi(cot)] Case. Angewandte Chemie, 2021, 133, 2620-2625.	1.6	21
60	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. Angewandte Chemie - International Edition, 2000, 39, 1786-1788.	7.2	20
61	Surface effects on a photochromic spin-crossover iron(ii) molecular switch adsorbed on highly oriented pyrolytic graphite. Nanoscale, 2019, 11, 20006-20014.	2.8	20
62	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.	2.9	19
63	Slow Magnetic Relaxation in Chiral Helicene-Based Coordination Complex of Dysprosium. Magnetochemistry, 2017, 3, 2.	1.0	19
64	On the importance of the biquadratic terms in exchange coupled systems: A post-HF investigation. Inorganica Chimica Acta, 2008, 361, 4153-4156.	1.2	18
65	Highly Axial Magnetic Anisotropy in a N₃O₅ Dysprosium(III) Coordination Environment Generated by a Merocyanine Ligand. Chemistry - A European Journal, 2016, 22, 15222-15226.	1.7	18
66	Magnetic Cationic Copper(II) Chains and a Mononuclear Cobalt(II) Complex Containing [Ln(hfac)₄]^â Blocks as Counterions. Inorganic Chemistry, 2019, 58, 1976-1987.	1.9	18
67	On the kinetics and thermodynamics of Sâ€“X (XÂ=ÂH, CH3, SCH3, COCH3, and CN) cleavage in the formation of self-assembled monolayers of alkylthiols on Au(111). Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	17
68	Computational Studies on SAMs of {Mn₆} SMMs on Au(111): Do Properties Change upon Grafting?. Journal of Physical Chemistry C, 2013, 117, 7186-7190.	1.5	16
69	DFT magnetic characterization of a Fe₄SMMs series: from isotropic exchange interactions to multi-spin zero field splitting. Journal of Materials Chemistry C, 2014, 2, 8333-8343.	2.7	16
70	Diâ€•and Triphosphate Recognition and Sensing with Monoâ€•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.	1.7	16
71	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.	1.2	15
72	Study of three new halogenated oxoquinolinecarbohydrazide N-phosphonate derivatives as corrosion inhibitor for mild steel in acid environment. Surfaces and Interfaces, 2020, 21, 100773.	1.5	15

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73	Temperature Dependence of Spinâ€“Phonon Coupling in [VO(acac)₂]: A Computational and Spectroscopic Study. Journal of Physical Chemistry C, 2021, 125, 22100-22110.	1.5	15
74	A dinuclear copper(II) complex with a Cu(O, Nâ€“O)Cu bridging core: structural and magnetic (experimental and density functional theory) studies. Inorganica Chimica Acta, 2004, 357, 2150-2156.	1.2	14
75	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.	1.2	14
76	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.	1.0	13
77	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.	3.2	13
78	DFT Description of the Electronic Structure and Spectromagnetic Properties of Strongly Correlated Electronic Systems: NiII, CuII and ZnIIo-Dioxolene Complexes. Chemistry - A European Journal, 2004, 10, 1472-1480.	1.7	11
79	Solution structure of a pentachromium(<scp>ii</scp>) single molecule magnet from DFT calculations, isotopic labelling and multinuclear NMR spectroscopy. Dalton Transactions, 2018, 47, 585-595.	1.6	11
80	Density Functional Description of the Early Stages of the Dioxygenation of [(MeC(CH2PPh2)3)M(catecholate)]+Complexes [M = Co(III), Ir(III)]:Â Toward a Rationalization of the Catalytic Mechanism of Ring-Opening Dioxygenases. Inorganic Chemistry, 2000, 39, 1418-1425.	1.9	10
81	Magnetic and Optical Properties of Cu(II)â˜Bis(oxamato) Complexes:â€‰ Combined Quantum Chemical Density Functional Theory and Vibrational Spectroscopy Studies. Journal of Physical Chemistry B, 2008, 112, 5585-5593.	1.2	10
82	Quantitative and Chemically Intuitive Evaluation of the Nature of Mâ˜L Bonds in Paramagnetic Compounds: Application of EDAâ€NOCV Theory to Spin Crossover Complexes. Chemistry - A European Journal, 2020, 26, 13677-13685.	1.7	9
83	Magnetic anisotropy on demand exploiting high-pressure as remote control: an ab initio proof of concept. Dalton Transactions, 2021, 50, 10621-10628.	1.6	9
84	UHV deposition and characterization of a mononuclear iron(III) Î²-diketonate complex on Au(111). Beilstein Journal of Nanotechnology, 2014, 5, 2139-2148.	1.5	8
85	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.	1.5	8
86	The disclosure of mesoscale behaviour of a 3d-SMM monolayer on Au(111) through a multilevel approach. Nanoscale, 2018, 10, 4096-4104.	2.8	8
87	An Oxalate-Bridged Copper(II) Complex Combining Monodentate Benzoate, 2,2â€²-bipyridine and Aqua Ligands: Synthesis, Crystal Structure and Investigation of Magnetic Properties. Molecules, 2020, 25, 1898.	1.7	8
88	Chemisorption of nitronylâ€“nitroxide radicals on gold surface: an assessment of morphology, exchange interaction and decoherence time. Nanoscale, 2021, 13, 7613-7621.	2.8	8
89	Accurate prediction of pressure and temperature T_{1/2} variation in solid state spin crossover by ab initio methods: the [Co^{II}(dpzca)₂] case. Journal of Materials Chemistry C, 2021, 9, 14256-14268.	2.7	7
90	Hetero-tri-spin systems: an alternative stairway to the Single Molecule Magnets heaven?. Dalton Transactions, 2021, 50, 15961-15972.	1.6	7

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91	Engineering Chemisorption of Fe₄ Singleâ€Molecule Magnets on Gold. Advanced Materials Interfaces, 2021, 8, 2101182.	1.9	7
92	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, 3015-3023.	1.7	6
93	A Dy₄ Cubane: A New Member in the Singleâ€Molecule Toroics Family. Angewandte Chemie, 2018, 130, 17335-17339.	1.6	5
94	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.	0.3	4
95	Quantitative Assessment of Ligand Substituent Effects on Ïƒâ€•and Ï€â€Contributions to Feâ^'N Bonds in Spin Crossover Fe^{II}Complexes. Chemistry - A European Journal, 2022, 28, .	1.7	4
96	Redox-Active Dysprosium Single-Molecule Magnet: Spectro-Electrochemistry and Theoretical Investigations. Magnetochemistry, 2019, 5, 46.	1.0	3
97	On the kinetics and thermodynamics of Sâ€“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.	0.0	0