

Federico Totti

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97
papers

3,519
citations

30
h-index

56
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100
ext. papers

4,017
ext. citations

7.5
avg, IF

5.25
L-index

#	Paper	IF	Citations
97	Quantum tunnelling of the magnetization in a monolayer of oriented single-molecule magnets. <i>Nature</i> , 2010 , 468, 417-21	50.4	515
96	The role of anharmonic phonons in under-barrier spin relaxation of single molecule magnets. <i>Nature Communications</i> , 2017 , 8, 14620	17.4	215
95	Density Functional Calculations of Magnetic Exchange Interactions in Polynuclear Transition Metal Complexes. <i>Inorganic Chemistry</i> , 1997 , 36, 5022-5030	5.1	203
94	On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems: The Case of the Ferromagnetic Copper(II) μ_2 -Azido Bridged Complexes. <i>Inorganic Chemistry</i> , 1999 , 38, 1996-2004	5.1	154
93	Density functional studies on the exchange interaction of a dinuclear Gd(III)-Cu(II) complex: method assessment, magnetic coupling mechanism and magneto-structural correlations. <i>Dalton Transactions</i> , 2009 , 3153-61	4.3	129
92	Intra-molecular origin of the spin-phonon coupling in slow-relaxing molecular magnets. <i>Chemical Science</i> , 2017 , 8, 6051-6059	9.4	112
91	Assessment of a Combined QM/MM Approach for the Study of Large Nitroxide Systems in Vacuo and in Condensed Phases. <i>Journal of the American Chemical Society</i> , 1998 , 120, 7069-7078	16.4	94
90	A Few Comments on the Application of Density Functional Theory to the Calculation of the Magnetic Structure of Oligo-Nuclear Transition Metal Clusters. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 144-54	6.4	88
89	Roles of Bridging Ligand Topology and Conformation in Controlling Exchange Interactions between Paramagnetic Molybdenum Fragments in Dinuclear and Trinuclear Complexes. <i>Inorganic Chemistry</i> , 1997 , 36, 3447-3454	5.1	85
88	Strong ferromagnetic interactions in [V(8)O(14)(H ₂ taci)(2)]: an unprecedented large spin ground state for a vanadyl cluster. <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 3436-9	16.4	74
87	Density Functional Modeling of Long Range Magnetic Interactions in Binuclear Oxomolybdenum(V) Complexes. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 10545-10551	2.8	65
86	Tetranuclear grid-like copper(II) complexes with pyrazolate bridges: syntheses, structures, magnetic and EPR spectroscopic properties. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999 , 339-348		63
85	Giant spin-phonon bottleneck effects in evaporable vanadyl-based molecules with long spin coherence. <i>Dalton Transactions</i> , 2016 , 45, 16635-16643	4.3	61
84	DFT description of the magnetic structure of polynuclear transition-metal clusters: The complexes [Cu(bpca) ₂ (H ₂ O) ₂][Cu(NO ₃) ₂] ₂ , (bpca = Bis(2-pyridylcarbonyl)amine), and [Cu(DBSQ)(C ₂ H ₅ O)] ₂ , (DBSQ = 3,5-di-tert-butyl-semiquinonato). <i>International Journal of Quantum Chemistry</i> , 2005 , 101, 819-825	2.1	60
83	Magnetic bistability in a submonolayer of sublimated Fe ₄ single-molecule magnets. <i>Nano Letters</i> , 2015 , 15, 535-41	11.5	57
82	Magnetic Slow Relaxation in a Metal-Organic Framework Made of Chains of Ferromagnetically Coupled Single-Molecule Magnets. <i>Chemistry - A European Journal</i> , 2018 , 24, 6983-6991	4.8	54
81	Relaxation Dynamics and Magnetic Anisotropy in a Low-Symmetry Dy(III) Complex. <i>Chemistry - A European Journal</i> , 2016 , 22, 5552-62	4.8	52

80	Magnetic fingerprint of individual Fe ₄ molecular magnets under compression by a scanning tunnelling microscope. <i>Nature Communications</i> , 2015 , 6, 8216	17.4	46
79	Molecular magnets and surfaces: A promising marriage. A DFT insight. <i>Coordination Chemistry Reviews</i> , 2015 , 289-290, 357-378	23.2	46
78	Density Functional Modeling of Double Exchange Interactions in Transition Metal Complexes. Calculation of the Ground and Excited State Properties of [Fe ₂ (OH) ₃ (tmtacn) ₂] ²⁺ . <i>Journal of the American Chemical Society</i> , 1998 , 120, 8357-8365	16.4	45
77	Dynamic control of magnetic nanowires by light-induced domain-wall kickoffs. <i>Nature Materials</i> , 2013 , 12, 202-6	27	42
76	Improved slow magnetic relaxation in optically pure helicene-based Dy single molecule magnets. <i>Chemical Communications</i> , 2016 , 52, 14474-14477	5.8	41
75	Electrochemical and Magnetic Exchange Interactions in Trinuclear Chain Complexes Containing Oxo-Mo(V) Fragments as a Function of the Topology of the Bridging Ligand. <i>Inorganic Chemistry</i> , 1999 , 38, 365-369	5.1	41
74	A chimeric design of heterospin 2p-3d, 2p-4f, and 2p-3d-4f complexes using a novel family of paramagnetic dissymmetric compartmental ligands. <i>Chemical Communications</i> , 2017 , 53, 6504-6507	5.8	40
73	cis-Pt I ₂ (NH ₃) ₂ : a reappraisal. <i>Dalton Transactions</i> , 2015 , 44, 14896-905	4.3	40
72	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. <i>Dalton Transactions RSC</i> , 2001 , 1401-1414		36
71	Tunable Spin-Superconductor Coupling of Spin 1/2 Vanadyl Phthalocyanine Molecules. <i>Nano Letters</i> , 2018 , 18, 7955-7961	11.5	36
70	Covalency and magnetic anisotropy in lanthanide single molecule magnets: the DyDOTA archetype. <i>Chemical Science</i> , 2019 , 10, 7233-7245	9.4	35
69	DFT description of the magnetic properties and electron localization in dinuclear di-μ-oxo-bridged manganese complexes. <i>Chemistry - A European Journal</i> , 2002 , 8, 5019-27	4.8	31
68	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. <i>Inorganic Chemistry</i> , 2019 , 58, 13090-13101	5.1	30
67	Room temperature control of spin states in a thin film of a photochromic iron(II) complex. <i>Materials Horizons</i> , 2018 , 5, 506-513	14.4	30
66	A periodic mixed gaussians-plane waves DFT study on simple thiols on Au(111): adsorbate species, surface reconstruction, and thiols functionalization. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 3886-95	3.6	29
65	A Dy Cubane: A New Member in the Single-Molecule Toroids Family. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 17089-17093	16.4	29
64	Crystal and molecular structure and magnetic exchange properties of bis(di-μ-ethoxy-bis(3,5-di-tert-butylsemiquinonato)dicopper(II)) complex. A synergy between DFT and experimental magnetochemistry. <i>Inorganic Chemistry</i> , 2003 , 42, 8065-71	5.1	28
63	First coordination compounds based on a bis(imino nitroxide) biradical and 4f metal ions: synthesis, crystal structures and magnetic properties. <i>Dalton Transactions</i> , 2016 , 45, 2936-44	4.3	27

62	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. <i>Inorganic Chemistry</i> , 2000 , 39, 1288-93	5.1	27
61	A Complete View of Orbach and Raman Spin-Lattice Relaxation in a Dysprosium Coordination Compound. <i>Journal of the American Chemical Society</i> , 2021 , 143, 13633-13645	16.4	26
60	Mössbauer spectroscopy of a monolayer of single molecule magnets. <i>Nature Communications</i> , 2018 , 9, 480	17.4	25
59	Binuclear Lanthanide-Radical Complexes Featuring Two Centers with Different Magnetic and Luminescence Properties. <i>Inorganic Chemistry</i> , 2016 , 55, 11676-11684	5.1	25
58	Polyamine receptors containing dipyridine or phenanthroline units: clues for the design of fluorescent chemosensors for metal ions. <i>Chemistry - A European Journal</i> , 2009 , 15, 8049-63	4.8	25
57	Quantum dynamics of a single molecule magnet on superconducting Pb(111). <i>Nature Materials</i> , 2020 , 19, 546-551	27	24
56	Enhanced vapor-phase processing in fluorinated Fe ₄ single-molecule magnets. <i>Inorganic Chemistry</i> , 2013 , 52, 5897-905	5.1	24
55	Mononuclear, dinuclear, and pentanuclear [[N,S(thiolate)]iron(II)] complexes: nuclearity control, incorporation of hydroxide bridging ligands, and magnetic behavior. <i>Chemistry - A European Journal</i> , 2005 , 11, 7328-41	4.8	24
54	A Combined Ion Scattering, Photoemission, and DFT Investigation on the Termination Layer of a La _{0.7} Sr _{0.3} MnO ₃ Spin Injecting Electrode. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 13631-13637	3.8	22
53	Tetrathiafulvalene-Based Helicene Ligand in the Design of a Dysprosium Field-Induced Single-Molecule Magnet. <i>Inorganic Chemistry</i> , 2019 , 58, 52-56	5.1	22
52	Valence electronic structure of sublimated Fe ₄ single-molecule magnets: an experimental and theoretical characterization. <i>Journal of Materials Chemistry C</i> , 2014 , 2, 9599-9608	7.1	21
51	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. <i>Dalton Transactions</i> , 2003 , 36-45	4.3	21
50	A DFT exploration of the organization of thiols on Au(111): a route to self-assembled monolayer of magnetic molecules. <i>Journal of Materials Chemistry</i> , 2010 , 20, 10747		20
49	Theoretical Characterization of the Mechanism of Hg ^{II} Bond Cleavage by Halogenic Acids. <i>Organometallics</i> , 1996 , 15, 1465-1469	3.8	20
48	Lanthanide complexes involving multichelating TTF-based ligands. <i>Inorganic Chemistry Frontiers</i> , 2017 , 4, 604-617	6.8	18
47	Vanadyl phthalocyanines on graphene/SiC(0001): toward a hybrid architecture for molecular spin qubits. <i>Nanoscale Horizons</i> , 2019 , 4, 1202-1210	10.8	17
46	Modeling thiols on Au(111): Structural, thermodynamic and magnetic properties of simple thiols and thiol-radicals. <i>Superlattices and Microstructures</i> , 2009 , 46, 4-9	2.8	17
45	On the importance of the biquadratic terms in exchange coupled systems: A post-HF investigation. <i>Inorganica Chimica Acta</i> , 2008 , 361, 4153-4156	2.7	17

44	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). <i>Angewandte Chemie - International Edition</i> , 2000 , 39, 1786-1788	16.4	17
43	Theoretical Study of the Electronic Structure and of the Mercury-Carbon Bonding of Methylmercury(II) Compounds. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 12743-12750		17
42	Single molecule magnets grafted on gold: magnetic properties from ab initio molecular dynamics. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 7294-7304	7.1	16
41	On the kinetics and thermodynamics of S _X (X = H, CH ₃ , SCH ₃ , COCH ₃ , and CN) cleavage in the formation of self-assembled monolayers of alkylthiols on Au(111). <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	15
40	Magnetic Anisotropy Trends along a Full 4f-Series: The Effect. <i>Journal of the American Chemical Society</i> , 2021 , 143, 8108-8115	16.4	15
39	Magnetic Cationic Copper(II) Chains and a Mononuclear Cobalt(II) Complex Containing [Ln(hfac)] Blocks as Counterions. <i>Inorganic Chemistry</i> , 2019 , 58, 1976-1987	5.1	14
38	Exploring the Organometallic Route to Molecular Spin Qubits: The [CpTi(cot)] Case. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 2588-2593	16.4	14
37	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. <i>Chemistry - A European Journal</i> , 2016 , 22, 14890-14901	4.8	13
36	Surface effects on a photochromic spin-crossover iron(ii) molecular switch adsorbed on highly oriented pyrolytic graphite. <i>Nanoscale</i> , 2019 , 11, 20006-20014	7.7	13
35	DFT magnetic characterization of a Fe ₄ SMMs series: from isotropic exchange interactions to multi-spin zero field splitting. <i>Journal of Materials Chemistry C</i> , 2014 , 2, 8333-8343	7.1	13
34	Slow Magnetic Relaxation in Chiral Helicene-Based Coordination Complex of Dysprosium. <i>Magnetochemistry</i> , 2017 , 3, 2	3.1	13
33	Computational Studies on SAMs of {Mn ₆ } SMMs on Au(111): Do Properties Change upon Grafting?. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 7186-7190	3.8	13
32	Synthesis and characterization of new oligomeric and polymeric complexes based on the [CuII(bpca)] ⁺ unit [Hbpca = bis(2-pyridylcarbonyl)amine]. <i>Inorganica Chimica Acta</i> , 2011 , 376, 538-548	2.7	13
31	Comparison between post-Hartree-Fock and DFT methods for the study of strength and mechanism of cleavage of Hg(SINGLE BOND)C bond. <i>International Journal of Quantum Chemistry</i> , 1997 , 61, 361-367	2.1	13
30	Strong Ferromagnetic Interactions in [V ₈ O ₁₄ (H ₂ taci) ₂]: An Unprecedented Large Spin Ground State for a Vanadyl Cluster. <i>Angewandte Chemie</i> , 2004 , 116, 3518-3521	3.6	13
29	Highly Axial Magnetic Anisotropy in a N O Dysprosium(III) Coordination Environment Generated by a Merocyanine Ligand. <i>Chemistry - A European Journal</i> , 2016 , 22, 15222-15226	4.8	13
28	The Origin of Magnetic Anisotropy and Single-Molecule Magnet Behavior in Chromium(II)-Based Extended Metal Atom Chains. <i>Inorganic Chemistry</i> , 2020 , 59, 1763-1777	5.1	12
27	A dinuclear copper(II) complex with a Cu(O, N _D)Cu bridging core: structural and magnetic (experimental and density functional theory) studies. <i>Inorganica Chimica Acta</i> , 2004 , 357, 2150-2156	2.7	12

26	The Role of Anisotropic Exchange in Single Molecule Magnets: A CASSCF/NEVPT2 Study of the Fe ₄ SMM Building Block [Fe ₂ (OCH ₃) ₂ (dbm) ₄] Dimer. <i>Inorganics</i> , 2016 , 4, 28	2.9	12
25	DFT description of the electronic structure and spectromagnetic properties of strongly correlated electronic systems: NiII, CuII and ZnII o-dioxolene complexes. <i>Chemistry - A European Journal</i> , 2004 , 10, 1472-80	4.8	11
24	Probing Vibrational Symmetry Effects and Nuclear Spin Economy Principles in Molecular Spin Qubits. <i>Inorganic Chemistry</i> , 2021 , 60, 140-151	5.1	11
23	Magnetic and optical properties of Cu(II)-bis(oxamato) complexes: combined quantum chemical density functional theory and vibrational spectroscopy studies. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 5585-93	3.4	10
22	The Challenge of Thermal Deposition of Coordination Compounds: Insight into the Case of an Fe ₄ Single Molecule Magnet. <i>Chemistry of Materials</i> , 2016 , 28, 7693-7702	9.6	10
21	Density functional description of the early stages of the dioxygenation of [(MeC(CH ₂ PPh ₂) ₃)M(catecholate)] ⁺ complexes [M = Co(III), Ir(III)]: toward a rationalization of the catalytic mechanism of ring-opening dioxygenases. <i>Inorganic Chemistry</i> , 2000 , 39, 1418-25	5.1	8
20	Exploring the Organometallic Route to Molecular Spin Qubits: The [CpTi(cot)] Case. <i>Angewandte Chemie</i> , 2021 , 133, 2620-2625	3.6	8
19	Study of three new halogenated oxoquinolinecarbohydrazide N-phosphonate derivatives as corrosion inhibitor for mild steel in acid environment. <i>Surfaces and Interfaces</i> , 2020 , 21, 100773	4.1	7
18	UHV deposition and characterization of a mononuclear iron(III) Ediketonate complex on Au(111). <i>Beilstein Journal of Nanotechnology</i> , 2014 , 5, 2139-48	3	6
17	Density functional characterization of the chemoselective oxidation of catechol by using molecular oxygen: thermodynamics of the reaction between [(triphos)Ir(dtbc)] ⁺ and O ₂ . <i>Chemistry - A European Journal</i> , 2003 , 9, 3015-23	4.8	6
16	Solution structure of a pentachromium(ii) single molecule magnet from DFT calculations, isotopic labelling and multinuclear NMR spectroscopy. <i>Dalton Transactions</i> , 2018 , 47, 585-595	4.3	6
15	An Oxalate-Bridged Copper(II) Complex Combining Monodentate Benzoate, 2,2'-bipyridine and Aqua Ligands: Synthesis, Crystal Structure and Investigation of Magnetic Properties. <i>Molecules</i> , 2020 , 25,	4.8	5
14	Quantitative and Chemically Intuitive Evaluation of the Nature of M-L Bonds in Paramagnetic Compounds: Application of EDA-NOCV Theory to Spin Crossover Complexes. <i>Chemistry - A European Journal</i> , 2020 , 26, 13677-13685	4.8	5
13	Temperature Dependence of Spin-Phonon Coupling in [VO(acac)]: A Computational and Spectroscopic Study. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 22100-22110	3.8	5
12	The disclosure of mesoscale behaviour of a 3d-SMM monolayer on Au(111) through a multilevel approach. <i>Nanoscale</i> , 2018 , 10, 4096-4104	7.7	4
11	Toward Mesoscale Properties of Self-Assembled Monolayers of SMM on Au(111): An Integrated Ad Hoc FF and DFT Study. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 14774-14781	3.8	4
10	DFT Description of Mixed Valence Magnetic Systems. Mn(III)-Mn(IV) and Fe(II)-Fe(III) Complexes. <i>Molecular Crystals and Liquid Crystals</i> , 1999 , 335, 665-674		4
9	A Dy ₄ Cubane: A New Member in the Single-Molecule Toroids Family. <i>Angewandte Chemie</i> , 2018 , 130, 17335-17339	3.6	4

8	Chemisorption of nitronyl-nitroxide radicals on gold surface: an assessment of morphology, exchange interaction and decoherence time. <i>Nanoscale</i> , 2021 , 13, 7613-7621	7.7	4
7	Redox-Active Dysprosium Single-Molecule Magnet: Spectro-Electrochemistry and Theoretical Investigations. <i>Magnetochemistry</i> , 2019 , 5, 46	3.1	2
6	Innovative Characterization of Original Green Vanillin-derived Schiff Bases as Corrosion Inhibitors by A Synergic Approach Based on Electrochemistry, Microstructure, and Computational Analyses. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022 , 641, 128540	5.1	2
5	Accurate prediction of pressure and temperature T1/2 variation in solid state spin crossover by ab initio methods: the [Coll(dpzca)2] case. <i>Journal of Materials Chemistry C</i> ,	7.1	2
4	Magnetic anisotropy on demand exploiting high-pressure as remote control: an proof of concept. <i>Dalton Transactions</i> , 2021 , 50, 10621-10628	4.3	2
3	Engineering Chemisorption of Fe4 Single-Molecule Magnets on Gold. <i>Advanced Materials Interfaces</i> , 2021 , 8, 2101182	4.6	1
2	Hetero-tri-spin systems: an alternative stairway to the single molecule magnet heaven?. <i>Dalton Transactions</i> , 2021 , 50, 15961-15972	4.3	1
1	On the kinetics and thermodynamics of S _X (X = H, CH ₃ , SCH ₃ , COCH ₃ , and CN) cleavage in the formation of self-assembled monolayers of alkylthiols on Au(111). <i>Highlights in Theoretical Chemistry</i> , 2013 , 99-109		