Angela Rosa

List of Publications by Year
in descending order

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32 papers	1,547 citations	236925 25 h-index	414414 32 g-index
32 all docs	32 docs citations	32 times ranked	1783 citing authors

#	Article	IF	Citations
1	Electronic Spectra of M(CO)6(M = Cr, Mo, W) Revisited by a Relativistic TDDFT Approach. Journal of the American Chemical Society, 1999, 121, 10356-10365.	13.7	330
2	Effects of Porphyrin Core Saddling,meso-Phenyl Twisting, and Counterions on the Optical Properties ofmeso-Tetraphenylporphyrin Diacids:Â The [H4TPP](X)2(X = F, Cl, Br, I) Series as a Case Study. Journal of Physical Chemistry A, 2003, 107, 11468-11482.	2.5	131
3	Synergism of Porphyrin-Core Saddling and Twisting ofmeso-Aryl Substituents. Journal of Physical Chemistry A, 2006, 110, 5180-5190.	2.5	79
4	Excitation Energies of Metal Complexes with Time-dependent Density Functional Theory. Structure and Bonding, 2004, , 49-116.	1.0	74
5	Density Functional Study of the Photodissociation of Mn2(CO)10. Inorganic Chemistry, 1996, 35, 2886-2897.	4.0	64
6	Photophysics of Octabutoxy Phthalocyaninato-Ni(II) in Toluene:Â Ultrafast Experiments and DFT/TDDFT Studies. Journal of Physical Chemistry A, 2005, 109, 2078-2089.	2.5	55
7	Density Functional Study of Ground and Excited States of Mn2(CO)10. Inorganic Chemistry, 1995, 34, 3425-3432.	4.0	54
8	Electronic Structure, Chemical Bond, and Optical Spectra of Metal Bis(porphyrin) Complexes:Â A DFT/TDDFT Study of the Bis(porphyrin)M(IV) (M = Zr, Ce, Th) Series. Journal of the American Chemical Society, 2002, 124, 12319-12334.	13.7	54
9	Evidence for Tetraphenylporphyrin Monoacids. Inorganic Chemistry, 2007, 46, 5979-5988.	4.0	52
10	Is [FeO]²⁺ the Active Center Also in Iron Containing Zeolites? A Density Functional Theory Study of Methane Hydroxylation Catalysis by Fe-ZSM-5 Zeolite. Inorganic Chemistry, 2010, 49, 3866-3880.	4.0	52
11	Structural, Optical, and Photophysical Properties of Nickel(II) Alkylthioporphyrins:Â Insights from Experimental and DFT/TDDFT Studies. Inorganic Chemistry, 2005, 44, 6609-6622.	4.0	48
12	Near-Infrared-Emitting Phthalocyanines. A Combined Experimental and Density Functional Theory Study of the Structural, Optical, and Photophysical Properties of Pd(II) and Pt(II) Î±-Butoxyphthalocyanines. Inorganic Chemistry, 2011, 50, 1135-1149.	4.0	46
13	Effects of Benzoannulation and Î±-Octabutoxy Substitution on the Photophysical Behavior of Nickel Phthalocyanines:Â A Combined Experimental and DFT/TDDFT Study. Inorganic Chemistry, 2007, 46, 2080-2093.	4.0	43
14	Metal-to-Ligand Charge Transfer (MLCT) Photochemistry offac-Mn(Cl)(CO)3(H-DAB):Â A Density Functional Study. The Journal of Physical Chemistry, 1996, 100, 15346-15357.	2.9	39
15	Photodissociation of the Phosphine-Substituted Transition Metal Carbonyl Complexes Cr(CO)5L and Fe(CO)4L:Â A Theoretical Study. Journal of the American Chemical Society, 2003, 125, 3558-3567.	13.7	39
16	Synthesis, Structure, and Physicochemical Properties of ((Ethylsulfanyl)porphyrazinato)cobalt(II). Metalâ^'Ligand Bonds in Co(OESPz) and in Related Cobalt(II) Tetrapyrroles:Â Insights from a Density Functional Study. Inorganic Chemistry, 1999, 38, 1422-1431.	4.0	37
17	Carboranyl-porphyrazines and derivatives for boron neutron capture therapy: From synthesis to in vitro tests. Coordination Chemistry Reviews, 2013, 257, 2213-2231.	18.8	37
18	Synthesis and Liposome Insertion of a New Poly(carboranylalkylthio)porphyrazine to Improve Potentiality in Multiple-Approach Cancer Therapy. Journal of the American Chemical Society, 2007, 129, 2728-2729.	13.7	36

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19	Structural Properties of M(dmit)2-Based (M = Ni, Pd, Pt; dmit2-= 2-Thioxo-1,3-dithiole-4,5-dithiolato) Molecular Metals. Insights from Density Functional Calculations. Inorganic Chemistry, 1998, 37, 1368-1379.	4.0	35
20	Tetra-2,3-pyrazinoporphyrazines with Externally Appended Pyridine Rings. 6. Chemical and Redox Properties and Highly Effective Photosensitizing Activity for Singlet Oxygen Production of Penta- and Monopalladated Complexes in Dimethylformamide Solution. Inorganic Chemistry, 2008, 47, 8757-8766.	4.0	34
21	Porphyrin vs phthalocyanine metallomacrocycles based one-dimensional "molecular metals". Insights from density functional calculations. Inorganic Chemistry, 1993, 32, 5637-5639.	4.0	33
22	Density Functional Study of the Primary Photoprocesses of Manganese Pentacarbonyl Chloride (MnCl(CO)5). Inorganic Chemistry, 1997, 36, 1541-1551.	4.0	31
23	Reactivity of Compound II: Electronic Structure Analysis of Methane Hydroxylation by Oxoiron(IV) Porphyrin Complexes. Inorganic Chemistry, 2012, 51, 9833-9845.	4.0	29
24	Charge Effects on the Reactivity of Oxoiron(IV) Porphyrin Species: A DFT Analysis of Methane Hydroxylation by Polycationic Compound I and Compound II Mimics. ACS Catalysis, 2016, 6, 568-579.	11.2	27
25	Phenyl Derivative of Iron 5,10,15-Tritolylcorrole. Inorganic Chemistry, 2014, 53, 4215-4227.	4.0	26
26	Metal-to-Ligand Charge Transfer Photochemistry:Â Homolysis of the Mnâ^'Cl Bond in themer-Mn(Cl)(CO)3(Ï±-diimine) Complex and Its Absence in thefac-Isomer. Inorganic Chemistry, 1998, 37, 6244-6254.	4.0	20
27	Photophysical Behavior of Open-Shell First-Row Transition-Metal Octabutoxynaphthalocyanines: CoNc(OBu)₈ and CuNc(OBu)₈ as Case Studies. Inorganic Chemistry, 2008, 47, 4275-4289.	4.0	15
28	Nickel-macrocycle interaction in nickel(II) porphyrins and porphyrazines bearing alkylthio Î²-substituents: A combined DFT and XPS study. Journal of Porphyrins and Phthalocyanines, 2017, 21, 371-380.	0.8	12
29	The role of the metal ion in the photophysical behavior of Co(II), Ni(II), and Cu(II) octabutoxynaphthalocyanines: insights from ultra-fast time-resolved spectroscopy and DFT/TDDFT calculations. Journal of Porphyrins and Phthalocyanines, 2010, 14, 689-700.	0.8	5
30	Origin of the Enhanced Binding Capability toward Axial Nitrogen Bases of Ni(II) Porphyrins Bearing Electron-Withdrawing Substituents: An Electronic Structure and Bond Energy Analysis. Inorganic Chemistry, 2020, 59, 11528-11541.	4.0	4
31	On the photophysics of metallophthalocyanine-based photothermal sensitizers: Synergism between theory and experiment. Journal of Inorganic Biochemistry, 2008, 102, 406-413.	3.5	3
32	Bis(CBT)palladium(II) Derivatives (CBT = m-carborane-1-thiolate): Synthesis, Molecular Structure, and Physicochemical Properties of cis-[(bipy)Pd(CBT)₂] and trans-[(py)₂Pd(CBT)₂]. Inorganic Chemistry, 2021, 60, 10478-10491.	4.0	3