Fernando Mendizabal

List of Publications by Year
in descending order

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Version: 2024-02-01

48 papers	1,716 citations	430874 18 h-index	276875 41 g-index
48 all docs	48 docs citations	48 times ranked	1446 citing authors

#	Article	IF	Citations
1	Closed-shell d¹⁰â€“d¹⁰ in [AuCl(CNR)]_n and [AuCl(CO)]_n (n = 1, 2; R = â€“H, â€“CH₃, â€“Cy) complexes: quantum chemistry study of their electronic and optical properties. RSC Advances, 2022, 12, 7516-7528.	3.6	1
2	Designing boron and metal complexes for fluoride recognition: a computational perspective. Physical Chemistry Chemical Physics, 2021, 23, 22768-22778.	2.8	0
3	Exploration of the Activation Mechanism of the Epigenetic Regulator MLL3: A QM/MM Study. Biomolecules, 2021, 11, 1051.	4.0	3
4	Insights into the role of Dâ€Aâ€Ïâ€A type proâ€aromatic organic dyes with thieno[3,4â€b]pyrazine as A acceptor group into dyeâ€sensitized solarâ€cells. A TDâ€DFT/periodic DFT study. International Journal of Quantum Chemistry, 2020, 120, e26108.	2.0	6
5	Exploration of the Interaction Strength at the Interface of Anionic Chalcogen Anchors and Gold (111)-Based Nanomaterials. Nanomaterials, 2020, 10, 1237.	4.1	1
6	Electronic and optical properties of [Au(CH₃CSS)]₄ cluster. A quantum chemistry study. RSC Advances, 2020, 10, 33549-33557.	3.6	4
7	On the recognition of chloride, bromide and nitrate anions by anthraceneâ€“squaramide conjugated compounds: a computational perspective. New Journal of Chemistry, 2020, 44, 17831-17839.	2.8	9
8	Quantum chemistry simulation of the electronic properties in [Au(NH₃)₂]NO₃ and [Au(NCH)₂][AuCl₄] extended unsupported complexes. Molecular Simulation, 2020, 46, 521-529.	2.0	8
9	Theoretical exploration of the forces governing the interaction between goldâ€“phthalocyanine and gold surface clusters. RSC Advances, 2020, 10, 3895-3901.	3.6	7
10	Noncovalent interactions in inorganic supramolecular chemistry based in heavy metals. Quantum chemistry point of view. International Journal of Quantum Chemistry, 2019, 119, e25675.	2.0	27
11	Catalytic activity of iron phthalocyanine for the oxidation of thiocyanate and L-cysteine anchored on Au(111) clusters. Molecular Simulation, 2019, 45, 1447-1453.	2.0	3
12	Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. ChemCatChem, 2018, 10, 1052-1063.	3.7	14
13	Electronic structure and optical properties calculation of Zn-porphyrin with N-annulated perylene adsorbed on TiO2 model for dye-sensitized solar cell applications: A DFT/TD-DFT study. Computational Materials Science, 2017, 126, 514-527.	3.0	17
14	Electronic and optical properties of metalloporphyrins of zinc on TiO₂ cluster in dye-sensitized solar-cells (DSSC). A quantum chemistry study. RSC Advances, 2017, 7, 42677-42684.	3.6	29
15	Calculations of the light absorption spectra of porphyrinoid chromophores for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2016, 18, 27877-27884.	2.8	8
16	Catalytic aspects of metallophthalocyanines adsorbed on gold-electrode. Theoretical exploration of the binding nature role. Physical Chemistry Chemical Physics, 2016, 18, 29516-29525.	2.8	10
17	Theoretical exploration of seleno and tellurophenols as promising alternatives to sulfur ligands for anchoring to gold (111) materials. RSC Advances, 2016, 6, 4458-4468.	3.6	8
18	A comparative study between post-Hartreeâ€“Fock methods and density functional theory in closed-shell aurophilic attraction. Computational and Theoretical Chemistry, 2015, 1057, 74-79.	2.5	18

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19	Theoretical study on interactions of fluorinated organomercurials with arene and gold fragments. Physical Chemistry Chemical Physics, 2015, 17, 26417-26428.	2.8	5
20	Interaction of LD14 and TiO2 in dye-sensitized solar-cells (DSSC): A density functional theory study. Computational and Theoretical Chemistry, 2015, 1070, 117-125.	2.5	15
21	Interaction of YD2 and TiO2 in dye-sensitized solar cells (DSSCs): a density functional theory study. Journal of Molecular Modeling, 2015, 21, 226.	1.8	13
22	Theoretical study on electronic spectra and interaction in [Au3]-L-[Au3] (L = C6F6,Ag+) complexes. Journal of Molecular Modeling, 2013, 19, 1973-1979.	1.8	7
23	Theoretical insights into the adsorption of neutral, radical and anionic thiophenols on gold(111). Physical Chemistry Chemical Physics, 2013, 15, 20363.	2.8	25
24	Enhancement of the Catalytic Activity of Fe Phthalocyanine for the Reduction of O₂ Anchored to Au(111) via Conjugated Self-Assembled Monolayers of Aromatic Thiols As Compared to Cu Phthalocyanine. Journal of Physical Chemistry C, 2012, 116, 15329-15341.	3.1	69
25	Theoretical and Experimental Study of Bonding and Optical Properties of Self-Assembly Metallophthalocyanines Complexes on a Gold Surface. A Survey of the Substrateâ€“Surface Interaction.. Journal of Physical Chemistry C, 2011, 115, 23512-23518.	3.1	21
26	Theoretical study of the closed-shell d10â€“d10 Au(I)â€“Cu(I) attraction in complexes in extended unsupported chains. Computational and Theoretical Chemistry, 2011, 965, 163-167.	2.5	15
27	Theoretical study of {Au₃(CH₃Ñ£¾COCH₃)₃}_nÂ·{2,4,7â€trinitroâ€9â€fluorenone} (n = 1,2) complexes. International Journal of Quantum Chemistry, 2010, 110, 1279-1286.	2.6	2
28	Theoretical study of the d10â€“s2 interaction between Au(I) and Tl(I) in the [AuCl(PH3)2]Tl+ hypothetical complex. Chemical Physics Letters, 2009, 479, 156-159.	2.6	4
29	Theoretical study of the electronic spectra of biâ€•and triâ€heteronuclear platinum complexes. International Journal of Quantum Chemistry, 2008, 108, 1164-1172.	2.0	6
30	Theoretical study of [Hg3(o-C6F4)3]nÂ·{benzene} (n=1, 2) complexes. Chemical Physics Letters, 2008, 463, 272-277.	2.6	11
31	Theoretical study on electronic spectra and aurophilic attraction in <mml:math altimg="si83.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/co	2.6	18
32	Complexes self-associate by hydrogen bonding and metallophilic attraction: Theoretical study. International Journal of Quantum Chemistry, 2006, 106, 906-912.	2.0	12
33	Theoretical study on the electronic spectrum of (M=Au(I), Ag(I); n=1â€“3) complexes. Computational and Theoretical Chemistry, 2006, 764, 187-194.	1.5	6
34	Theoretical study of the interaction d10â€“s2 between Pt(0) and Tl(I) on the [Pt(PH3)3Tl]+ complex. Chemical Physics Letters, 2005, 412, 477-481.	2.6	11
35	Theoretical study of the electronic spectrum of binuclear gold(I) complexes. International Journal of Quantum Chemistry, 2005, 103, 34-44.	2.0	26
36	A Detailed Study of the Vapochromic Behavior of {Tl[Au(C6Cl5)2]}n. Inorganic Chemistry, 2004, 43, 3573-3581.	4.0	104

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37	Aurophilic attraction in binuclear complexes with Au(i) and Au(iii). A theoretical study. Physical Chemistry Chemical Physics, 2004, 6, 900-905.	2.8	82
38	Theoretical study of the d10â€“d8 interaction between Au(I) and Au(III) on the cis/trans-[PH3Au(I)C(L)î˜…C(L)Au(III)(R)2PH3] (R=â€“H, â€“CH3; L=â€“H, â€“CH3) systems. Chemical Physics Letters, 2003, 382, 92-99.	2.6	28
39	Theoretical and Photoluminescence Studies on the d10â€“s2 Aulâ€“Tll Interaction in Extended Unsupported Chains. Chemistry - A European Journal, 2003, 9, 456-465.	3.3	75
40	Aurophilic attraction: the additivity and the combination with hydrogen bonds. Chemical Physics Letters, 2003, 370, 733-740.	2.6	48
41	Mixed Gold(I)â^'Gold(III) Complexes with Bridging Selenido Ligands. Theoretical Studies of the Gold(I)â^'Gold(III) Interactions. Organometallics, 2001, 20, 4812-4818.	2.3	38
42	Theoretical Study of Goldâ^'Carbonyls Interaction in Au(CO)n(n= 1â^'3) Complexes. Organometallics, 2001, 20, 261-265.	2.3	27
43	Polynuclear Gold Complexes with Bridging Selenido Ligands. Theoretical Studies of Goldâ^'Gold Interactions. Organometallics, 2000, 19, 4985-4994.	2.3	34
44	Theoretical study of the Au-ethylene interaction. International Journal of Quantum Chemistry, 1999, 73, 317-324.	2.0	13
45	Theory of d10â^'d10Closed-Shell Attraction. III. Rings. Inorganic Chemistry, 1998, 37, 3018-3025.	4.0	207
46	Theory of the d¹⁰â€“d¹⁰ Closedâ€Shell Attraction: 1. Dimers Near Equilibrium. Chemistry - A European Journal, 1997, 3, 1451-1457.	3.3	430
47	Theory of the d¹⁰â€“d¹⁰ Closedâ€Shell Attraction: 2. Longâ€Distance Behaviour and Nonadditive Effects in Dimers and Trimers of Type [(xâ€Auâ€L)_n] (n = 2, 3; X = Cl, I,) Tj ET Q q 1 1 0	3.3	784314
48	Quantum chemistry study in metallophilic interactions on complexes based in Au(I)-Pb(II) and Au(I)-Bi(III). Molecular Simulation, 0, , 1-11.	2.0	0