Fernando Mendizabal

List of Publications by Year
in descending order

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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	Theory of the d¹⁰â€“d¹⁰ Closedâ€Shell Attraction: 1. Dimers Near Equilibrium. Chemistry - A European Journal, 1997, 3, 1451-1457.	3.3	430
2	Theory of d10â^'d10Closed-Shell Attraction. III. Rings. Inorganic Chemistry, 1998, 37, 3018-3025.	4.0	207
3	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 0 rg	3.0	178
4	A Detailed Study of the Vapochromic Behavior of {Tl[Au(C6Cl5)2]}n. Inorganic Chemistry, 2004, 43, 3573-3581.	4.0	104
5	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
6	Theoretical and Photoluminescence Studies on the d10â€“s2 Auâ€“Tll Interaction in Extended Unsupported Chains. Chemistry - A European Journal, 2003, 9, 456-465.	3.3	75
7	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
8	Aurophilic attraction: the additivity and the combination with hydrogen bonds. Chemical Physics Letters, 2003, 370, 733-740.	2.6	48
9	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
10	Polynuclear Gold Complexes with Bridging Selenido Ligands. Theoretical Studies of Goldâ^'Gold Interactions. Organometallics, 2000, 19, 4985-4994.	2.3	34
11	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
12	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
13	Theoretical Study of Goldâ^'Carbonyls Interaction in Au(CO)n(n= 1â^'3) Complexes. Organometallics, 2001, 20, 261-265.	2.3	27
14	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
15	Theoretical study of the electronic spectrum of binuclear gold(I) complexes. International Journal of Quantum Chemistry, 2005, 103, 34-44.	2.0	26
16	Theoretical insights into the adsorption of neutral, radical and anionic thiophenols on gold(111). Physical Chemistry Chemical Physics, 2013, 15, 20363.	2.8	25
17	Theoretical and Experimental Study of Bonding and Optical Properties of Self-Assembly Metallophthalocyanines Complexes on a Gold Surface. A Survey of the Substrateâ€“Surface 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	3.1	21
18		2.6	18

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19	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
20	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
21	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
22	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
23	Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. ChemCatChem, 2018, 10, 1052-1063.	3.7	14
24	Theoretical study of the Au-ethylene interaction. International Journal of Quantum Chemistry, 1999, 73, 317-324.	2.0	13
25	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
26	Complexes self-associate by hydrogen bonding and metallophilic attraction: Theoretical study. International Journal of Quantum Chemistry, 2006, 106, 906-912.	2.0	12
27	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
28	Theoretical study of [Hg3(o-C6F4)3]nÂ·{benzene} (n=1, 2) complexes. Chemical Physics Letters, 2008, 463, 272-277.	2.6	11
29	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
30	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
31	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
32	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
33	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
34	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
35	Theoretical exploration of the forces governing the interaction between goldâ€“phthalocyanine and gold surface clusters. RSC Advances, 2020, 10, 3895-3901.	3.6	7
36	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

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37	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
38	Theoretical study of {Au₃(CH₃NÏ£¾COCH₃)₃}_nÂ·{2,4,7â€trinitroâ€9â€fluorenone} (n = 1,2) complexes. International Journal of Quantum Chemistry, 2010, 110, 1279-1286.	2.0	6
39	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
40	Theoretical study on interactions of fluorinated organomercurials with arene and gold fragments. Physical Chemistry Chemical Physics, 2015, 17, 26417-26428.	2.8	5
41	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
42	Electronic and optical properties of [Au(CH₃CSS)]₄ cluster. A quantum chemistry study. RSC Advances, 2020, 10, 33549-33557.	3.6	4
43	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
44	Exploration of the Activation Mechanism of the Epigenetic Regulator MLL3: A QM/MM Study. Biomolecules, 2021, 11, 1051.	4.0	3
45	Exploration of the Interaction Strength at the Interface of Anionic Chalcogen Anchors and Gold (111)-Based Nanomaterials. Nanomaterials, 2020, 10, 1237.	4.1	1
46	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
47	Designing boron and metal complexes for fluoride recognition: a computational perspective. Physical Chemistry Chemical Physics, 2021, 23, 22768-22778.	2.8	0
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