Ana Martinez

List of Publications by Year in Descending Order

147 papers	3,033 citations	31 h-index	47 g-index
151 ext. papers	3,296 ext. citations	3.4 avg, IF	5.63 L-index

#	Paper	IF	Citations
147	Different anchoring ligands for Ru complexes dyes and the effect on the performance of ZnO-based Dye-Sensitized Solar Cell (DSSC): A computational study. *Computational and Theoretical Chemistry*, **2022**, 1209, 113627	2	0
146	Analyzing the interaction energy between dopaminergic agents and DRD2: Is there any difference between risperidone (antagonist), aripiprazole (partial agonist) and pramipexole (agonist)?. *Computational and Theoretical Chemistry*, **2021**, 1197, 113125	2	5
145	Copper and neurodegenerative disorders: potential drugs for possible successful treatment. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	1
144	Electron Donor-Acceptor Capacity of Selected Pharmaceuticals against COVID-19. *Antioxidants*, **2021**, 10,	7.1	3
143	Interaction of graphene with antipsychotic drugs: Is there any charge transfer process?. *Journal of Computational Chemistry*, **2021**, 42, 60-65	3.5	6
142	Identification of the preferential CO and SO adsorption sites within NOTT-401. *Physical Chemistry Chemical Physics*, **2021**, 23, 1454-1463	3.6	2
141	Main interactions of dopamine and risperidone with the dopamine D2 receptor. *Physical Chemistry Chemical Physics*, **2021**, 23, 14224-14230	3.6	0
140	Electron Donor-Acceptor Properties of Different Muscarinic Ligands: On the Road to Control Schizophrenia. *Journal of Chemical Information and Modeling*, **2021**, 61, 5117-5124	6.1	
139	New information of dopaminergic agents based on quantum chemistry calculations. *Scientific Reports*, **2020**, 10, 21581	4.9	8
138	A detailed description of the CO molecule adsorbed in InOF-1. *Physical Chemistry Chemical Physics*, **2020**, 22, 7969-7974	3.6	3
137	Confined benzene within InOF-1: contrasting CO and SO capture behaviours. *Dalton Transactions*, **2020**, 49, 2786-2793	4.3	4
136	Fluorometric detection of iodine by MIL-53(Al)-TDC. *Dalton Transactions*, **2020**, 49, 6572-6577	4.3	9
135	Dopamine antagonists for the treatment of drug addiction: PF-4363467 and related compounds. *European Journal of Chemistry*, **2020**, 11, 84-90	0.6	6
134	ZnO Nanowires/N719 Dye With Different Aspect Ratio as a Possible Photoelectrode for Dye-Sensitized Solar Cells. *Frontiers in Chemistry*, **2020**, 8, 604092	5	2
133	Binding of multiple SO2 molecules to small gold cluster anions (AuN□AuNOH□N = 1-8). *International Journal of Quantum Chemistry*, **2019**, 119, e25987	2.1	2
132	High and energy-efficient reversible SO2 uptake by a robust Sc(III)-based MOF. *Journal of Materials Chemistry A*, **2019**, 7, 15580-15584	13	50
131	Relevance of hydrogen bonding in CO capture enhancement within InOF-1: an energy and vibrational analysis. *Dalton Transactions*, **2019**, 48, 8611-8616	4.3	8

130	CO capture enhancement for InOF-1: confinement of 2-propanol. *Dalton Transactions*, **2019**, 48, 5176-5182	4.3	7
129	A quantum chemical approach representing a new perspective concerning agonist and antagonist drugs in the context of schizophrenia and Parkinson's disease. *PLoS ONE*, **2019**, 14, e0224691	3.7	9
128	N719 Derivatives for Application in a Dye-Sensitized Solar Cell (DSSC): A Theoretical Study. *Journal of Physical Chemistry A*, **2019**, 123, 10930-10939	2.8	12
127	Confined toluene within InOF-1: CO capture enhancement.. *RSC Advances*, **2019**, 9, 32864-32872	3.7	5
126	A quantum chemical approach representing a new perspective concerning agonist and antagonist drugs in the context of schizophrenia and Parkinson disease **2019**, 14, e0224691		
125	A quantum chemical approach representing a new perspective concerning agonist and antagonist drugs in the context of schizophrenia and Parkinson disease **2019**, 14, e0224691		
124	A quantum chemical approach representing a new perspective concerning agonist and antagonist drugs in the context of schizophrenia and Parkinson disease **2019**, 14, e0224691		
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122	A quantum chemical approach representing a new perspective concerning agonist and antagonist drugs in the context of schizophrenia and Parkinson disease **2019**, 14, e0224691		
121	A quantum chemical approach representing a new perspective concerning agonist and antagonist drugs in the context of schizophrenia and Parkinson disease **2019**, 14, e0224691		
120	Greener synthesis of Cu-MOF-74 and its catalytic use for the generation of vanillin. *Dalton Transactions*, **2018**, 47, 4639-4645	4.3	46
119	On infinitenes Reliable calculation of and molecular modeling of lemniscate structured carotenoids. *Computational and Theoretical Chemistry*, **2018**, 1125, 133-141	2	3
118	Citric acid: A promising copper scavenger. *Computational and Theoretical Chemistry*, **2018**, 1133, 47-50	2	18
117	Cu, Ag and Au clusters as air pollutants hunters. *Computational and Theoretical Chemistry*, **2018**, 1130, 15-23	2	11
116	Confinement of HO and EtOH to enhance CO capture in MIL-53(Al)-TDC. *Dalton Transactions*, **2018**, 47, 9459-9465	4.3	12
115	A new free radical scavenging cascade involving melatonin and three of its metabolites (3OHM, AFMK and AMK). *Computational and Theoretical Chemistry*, **2018**, 1123, 111-118	2	23
114	How to identify promising metal scavengers? d-penicillamine with copper as a study case. *International Journal of Quantum Chemistry*, **2018**, 118, e25457	2.1	10
113	Copper or free radical scavenger?. *Computational and Theoretical Chemistry*, **2017**, 1104, 1-11	2	14

112	Confinement of alcohols to enhance CO2 capture in MIL-53(Al). *RSC Advances*, **2017**, 7, 24833-24840	3.7	18
111	Synthesis and properties of Bi5Nb3O15 thin films prepared by dual co-sputtering. *Journal of Alloys and Compounds*, **2017**, 695, 3704-3713	5.7	7
110	Structure stability of HKUST-1 towards water and ethanol and their effect on its CO capture properties. *Dalton Transactions*, **2017**, 46, 9192-9200	4.3	72
109	Silybin interacting with Cu 4 , Ag 4 and Au 4 clusters: Do these constitute antioxidant materials?. *Computational and Theoretical Chemistry*, **2017**, 1112, 1-9	2	12
108	How the presence of metal atoms and clusters can modify the properties of Silybin? A computational prediction. *Computational and Theoretical Chemistry*, **2017**, 1099, 174-184	2	12
107	Free radicals interacting with Cu, Ag and Au clusters. *Computational and Theoretical Chemistry*, **2017** , 1120, 24-33	2	11
106	Free radical scavenger properties of metal-fullerenes: C60 and C82 with Cu, Ag and Au (atoms and tetramers). *Computational and Theoretical Chemistry*, **2017**, 1115, 127-135	2	17
105	CO2 capture enhancement in InOF-1 via the bottleneck effect of confined ethanol. *Chemical Communications*, **2016**, 52, 10273-6	5.8	35
104	Reactivity Indexes of Fullerene and Bismullene Mixed Clusters: How the Intruders Modify the Properties. *Journal of Physical Chemistry A*, **2016**, 120, 8680-8685	2.8	5
103	Is Silybin the Best Free Radical Scavenger Compound in Silymarin?. *Journal of Physical Chemistry B*, **2016**, 120, 4568-78	3.4	13
102	Lycopene, oxidative cleavage derivatives and antiradical activity. *Computational and Theoretical Chemistry*, **2016**, 1077, 92-98	2	7
101	Age-Related Differences in the Gastrointestinal Microbiota of Chinstrap Penguins (Pygoscelis antarctica). *PLoS ONE*, **2016**, 11, e0153215	3.7	47
100	The influence of the carbohydrate anomeric linkage on the free radical scavenging activity of enzymatically-synthesized phenolic glycosides. *RSC Advances*, **2016**, 6, 45452-45461	3.7	2
99	Astaxanthin interacting with metal clusters: free radical scavenger and photovoltaic materials. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	3
98	Incorporation of novel azobenzene dyes bearing oligo(ethylene glycol) spacers into first generation dendrimers. *Dyes and Pigments*, **2015**, 116, 1-12	4.6	8
97	Antiradical capacity of ommochromes. *Journal of Molecular Modeling*, **2015**, 21, 220	2	16
96	Gold as an intruder in ZnO nanowires. *Physical Chemistry Chemical Physics*, **2015**, 17, 21525-32	3.6	8
95	Silybin and 2,3-Dehydrosilybin Flavonolignans as Free Radical Scavengers. *Journal of Physical Chemistry B*, **2015**, 119, 11597-606	3.4	15

94	Which Is The Best Sandwich Compound? Hexaphenylbenzene Substituted By Sandwich Compounds Bearing Sc, Cr, and Fe. *Journal of Physical Chemistry A*, **2015**, 119, 11523-31	2.8	8
93	Theoretical study of novel azo-tetraphenylporphyrins: potential photovoltaic materials. *Journal of Physical Chemistry A*, **2014**, 118, 197-207	2.8	4
92	New free radicals to measure antiradical capacity: a theoretical study. *Journal of Physical Chemistry B*, **2014**, 118, 10092-100	3.4	2
91	Free radical scavenging properties of phytofluene and phytoene isomers as compared to lycopene: a combined experimental and theoretical study. *Journal of Physical Chemistry B*, **2014**, 118, 9819-25	3.4	34
90	Structural evolution of small gold clusters doped by one and two boron atoms. *Journal of Computational Chemistry*, **2014**, 35, 2288-96	3.5	44
89	Gold-bismuth clusters. *Journal of Physical Chemistry A*, **2014**, 118, 5894-902	2.8	6
88	The effect of copper on the color of shrimps: redder is not always healthier. *PLoS ONE*, **2014**, 9, e107673	3.7	22
87	Design of novel luminescent porphyrins bearing donor–acceptor groups. *Journal of Porphyrins and Phthalocyanines*, **2014**, 18, 209-220	1.8	8
86	Boron as intruder in planar gold clusters. How does its presence modify reactivity?. *Computational and Theoretical Chemistry*, **2013**, 1021, 35-40	2	5
85	Iron, cadmium, and chromium in seagrass (Thalassia testudinum) from a coastal nature reserve in karstic Yucatán. *Environmental Monitoring and Assessment*, **2013**, 185, 7591-603	3.1	15
84	Keto, thione, selone, and tellone carotenoids: Changing antioxidants to antireductants. *Canadian Journal of Chemistry*, **2013**, 91, 621-627	0.9	6
83	Cis carotenoids: colorful molecules and free radical quenchers. *Journal of Physical Chemistry B*, **2013**, 117, 4050-61	3.4	20
82	Theoretical study of novel porphyrins bearing electron donor–acceptor groups. *International Journal of Quantum Chemistry*, **2013**, 113, 1376-1383	2.1	5
81	Synthesis and characterization of novel dendrons bearing amino-nitro-substituted azobenzene units and oligo(ethylene glycol) spacers: thermal, optical properties, Langmuir blodgett films and liquid-crystalline behaviour. *Molecules*, **2013**, 18, 1502-27	4.8	9
80	Electron uptake by classical electron donators: astaxanthin and carotenoid aldehydes. *Tetrahedron Letters*, **2012**, 53, 4522-4525	2	9
79	Dinuclear copper complexes with imidazole derivative ligands: a theoretical study related to catechol oxidase activity. *Journal of Physical Chemistry B*, **2012**, 116, 8038-44	3.4	21
78	The longest polyene. *Organic Letters*, **2012**, 14, 5496-8	6.2	19
77	Carbohydrates and their free radical scavenging capability: a theoretical study. *Journal of Physical Chemistry B*, **2012**, 116, 9668-75	3.4	65

76	Theoretical Study of the Electronic Properties of Silicon Nanocrystals Partially Passivated with Cl and F. *Journal of Physical Chemistry C*, **2012**, 116, 3988-3994	3.8	26
75	Capsaicin, a tasty free radical scavenger: mechanism of action and kinetics. *Journal of Physical Chemistry B*, **2012**, 116, 1200-8	3.4	75
74	The metal cation chelating capacity of astaxanthin. Does this have any influence on antiradical activity?. *Molecules*, **2012**, 17, 1039-54	4.8	26
73	Is the donor□cceptor electronegativity a good indicator for the surface enhanced Raman scattering (SERS)?. *International Journal of Quantum Chemistry*, **2012**, 112, 3516-3524	2.1	6
72	Xanthones as antioxidants: a theoretical study on the thermodynamics and kinetics of the single electron transfer mechanism. *Food and Function*, **2012**, 3, 442-50	6.1	33
71	Geographic variation in beak colouration in gentoo penguins Pygoscelis papua. *Polar Biology*, **2012**, 35, 725-731	2	6
70	Non-conventional hydrogen bonds: pterins-metal anions. *Physical Chemistry Chemical Physics*, **2011**, 13, 12775-84	3.6	8
69	Free radical scavenger properties of □-mangostin: thermodynamics and kinetics of HAT and RAF mechanisms. *Journal of Physical Chemistry B*, **2011**, 115, 12591-8	3.4	73
68	Photoelectron and computational studies of the copper-nucleoside anionic complexes, Cu(-)(cytidine) and Cu(-)(uridine). *Journal of Chemical Physics*, **2011**, 134, 054318	3.9	2
67	Phenylpropanoid glycoside analogues: enzymatic synthesis, antioxidant activity and theoretical study of their free radical scavenger mechanism. *PLoS ONE*, **2011**, 6, e20115	3.7	35
66	Negative ion photoelectron spectroscopy of the copper-aspartic acid anion and its hydrated complexes. *Journal of Chemical Physics*, **2010**, 133, 084303	3.9	1
65	Free Radical Scavenging Activity of Ultrashort Single-Walled Carbon Nanotubes with Different Structures through Electron Transfer Reactions. *Journal of Physical Chemistry C*, **2010**, 114, 8184-8191	3.8	57
64	Size Matters, but Is Being Planar of Any Relevance? Electron Donor□Acceptor Properties of Neutral Gold Clusters up to 20 Atoms. *Journal of Physical Chemistry C*, **2010**, 114, 21240-21246	3.8	33
63	On the Free Radical Scavenging Capability of Carboxylated Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2010**, 114, 6363-6370	3.8	27
62	Effect of Different Functional Groups on the Free Radical Scavenging Capability of Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2010**, 114, 14734-14739	3.8	25
61	Carotenoids can act as antioxidants by oxidizing the superoxide radical anion. *Physical Chemistry Chemical Physics*, **2010**, 12, 193-200	3.6	89
60	Electronic Structure of Silicon Nanocrystals Passivated with Nitrogen and Chlorine. *Journal of Physical Chemistry C*, **2010**, 114, 12427-12431	3.8	28
59	Influence of Point Defects on the Free-Radical Scavenging Capability of Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2010**, 114, 8302-8308	3.8	36

58	Electron donor–acceptor properties of metal atoms interacting with pterins. *New Journal of Chemistry*, **2010**, 34, 2988	3.6	8
57	Synthesis and characterization of a coupled binuclear Cu(I)/Cu(III) complex. *Journal of the American Chemical Society*, **2010**, 132, 10665-7	16.4	16
56	Are pterins able to modulate oxidative stress?. *Theoretical Chemistry Accounts*, **2010**, 127, 485-492	1.9	16
55	Theoretical study on the chemical fate of adducts formed through free radical addition reactions to carotenoids. *Theoretical Chemistry Accounts*, **2010**, 127, 595-603	1.9	32
54	Adenine–Au and adenine–uracil–Au. Non-conventional hydrogen bonds of the anions and donator–acceptor properties of the neutrals. *Computational and Theoretical Chemistry*, **2010**, 939, 34-43		8
53	Reactivity of aluminum cluster anions with ammonia: selective etching of Al11(-) and Al12(-). *Journal of Chemical Physics*, **2009**, 131, 184305	3.9	17
52	Theoretical study on the series of [Au(3)Cl (3)M (2)] complexes, with M = Li, Na, K, Rb, Cs. *Journal of Molecular Modeling*, **2009**, 15, 1165-73	2	9
51	Theoretical study of Au(I)–Ag(I) metallophilic attractions and luminescence of [Au2(carb)2Ag(η3,5-Ph2pz)] (with Ph = phenyl, pz = pyrazolate) and [Au(im)CH3(pz)Ag2(η3,5-H2pz)2] (with im = imidazole) complexes. *Computational and Theoretical Chemistry*, **2009**, 901, 232-242		8
50	Donator-acceptor map and work function for linear polyene-conjugated molecules. A density functional approximation study. *Journal of Physical Chemistry B*, **2009**, 113, 3212-7	3.4	25
49	Donator acceptor map of psittacofulvins and anthocyanins: are they good antioxidant substances?. *Journal of Physical Chemistry B*, **2009**, 113, 4915-21	3.4	58
48	Do anionic gold clusters modify conventional hydrogen bonds? The interaction of anionic Au(n) (n = 2-4) with the adenine-uracil base pair. *Journal of Physical Chemistry A*, **2009**, 113, 1134-40	2.8	31
47	What is important to prevent oxidative stress? A theoretical study on electron-transfer reactions between carotenoids and free radicals. *Journal of Physical Chemistry B*, **2009**, 113, 12113-20	3.4	71
46	Donator acceptor map for carotenoids, melatonin and vitamins. *Journal of Physical Chemistry A*, **2008**, 112, 9037-42	2.8	155
45	Nonconventional hydrogen bonds: a theoretical study of [uracil-L](-) (L = F, Cl, Br, I, Al, Ga, In) complexes. *Journal of Physical Chemistry A*, **2008**, 112, 10399-404	2.8	16
44	Theoretical study of neutral, anionic, and cationic uracil-Ag and uracil-Au systems: nonconventional hydrogen bonds. *Journal of Physical Chemistry A*, **2008**, 112, 2408-14	2.8	21
43	Theoretical study of cytosine-Al, cytosine-Cu and cytosine-Ag (neutral, anionic and cationic). *Journal of Physical Chemistry A*, **2008**, 112, 1033-9	2.8	29
42	Antiradical power of carotenoids and vitamin E: testing the hydrogen atom transfer mechanism. *Journal of Physical Chemistry B*, **2008**, 112, 16945-51	3.4	33
41	Reply to comment on construction of simplified models to simulate estrogenic disruptions by esters of 4-hydroxy benzoic acid (Parabens) by D. Godfrey. *Biophysical Chemistry*, **2008**, 138, 65	3.5	

40	Theoretical study of the novel sandwich compound [Au3Cl3Tr 2]2+. *Journal of Molecular Modeling*, **2008**, 14, 417-25	2	17
39	Construction of simplified models to simulate estrogenic disruptions by esters of 4-hydroxy benzoic acid (parabens). *Biophysical Chemistry*, **2008**, 137, 1-6	3.5	12
38	Ca, Cd, Zn, and their ions interacting with Cytosine: a theoretical study. *Journal of Physical Chemistry A*, **2007**, 111, 9931-9	2.8	21
37	Metal-Molecule Interactions To Produce Hydrogen: What Do They Have in Common?. *Journal of Chemical Theory and Computation*, **2007**, 3, 706-15	6.4	
36	Sequential addition of H2O, CH3OH, and NH3 to Al3O3-: a theoretical study. *Journal of Chemical Physics*, **2007**, 126, 024309	3.9	6
35	Electronic structure and luminescence of [AuS2PPh(OCH2CHCH2)]2 complex. *Computational and Theoretical Chemistry*, **2007**, 820, 141-147		25
34	Electron binding energies and Dyson orbitals of Al5Om- (m=3,4,5) and Al5O5H2-. *Journal of Chemical Physics*, **2007**, 127, 234302	3.9	9
33	Are structures with Al-H bonds represented in the photoelectron spectrum of Al3O4H2-?. *Journal of Chemical Physics*, **2006**, 124, 214304	3.9	15
32	Solvation of yttrium with ammonia revisited. Di-amide formation in the reaction of yttrium with ammonia. *Journal of Physical Chemistry A*, **2006**, 110, 1978-81	2.8	2
31	Deprotonated cytosine anions: a theoretical prediction of photoelectron spectra. *Journal of Physical Chemistry A*, **2006**, 110, 11174-7	2.8	10
30	A theoretical study of aromaticity in 1,2-diaza and 1,2-diphospha-cyclooctatetraenes and their role as ligands in organometallic compounds. *Computational and Theoretical Chemistry*, **2006**, 758, 49-52		2
29	Addition of water, methanol, and ammonia to Al3O3- clusters: reaction products, transition states, and electron detachment energies. *Journal of Chemical Physics*, **2005**, 122, 214309	3.9	21
28	Cluster size selectivity in the product distribution of ethene dehydrogenation on niobium clusters. *Journal of Physical Chemistry A*, **2005**, 109, 7046-56	2.8	14
27	Theoretical analysis of the fluxional behaviour of cyclooctatetraene Ru and Ni complexes. *Computational and Theoretical Chemistry*, **2005**, 732, 113-118		5
26	Bonding interactions of metal clusters [Mn (M= Cu, Ag, Au; n=1-4)] with ammonia. Are the metal clusters adequate as a model of surfaces?. *Journal of the Brazilian Chemical Society*, **2005**, 16, 337-344	1.5	11
25	Theoretical study of guanine-Cu and uracil-Cu (neutral, anionic, and cationic). Is it possible to carry out a photoelectron spectroscopy experiment?. *Journal of Chemical Physics*, **2005**, 123, 24311	3.9	23
24	Products of the addition of water molecules to Al3O3- clusters: structure, bonding, and electron binding energies in Al3O4H2-, Al3O5H4-, Al3O4H2, and Al3O5H4. *Journal of Chemical Physics*, **2004**, 120, 7955-62	3.9	16
23	Solvation of Al□uanine Complexes with NH3: A Theoretical Study. *Journal of Physical Chemistry A*, **2004**, 108, 5845-5850	2.8	8

22	Theoretical Study of the Dissociation of N2O in a Transition Metal Ion-Catalyzed Reaction. *Journal of Physical Chemistry B*, **2004**, 108, 8823-8829	3.4	31
21	Stabilization of an Unusual Tautomer of Guanine: Photoionization of Al□Guanine and Al□Guanine□(NH3)n. *Journal of Physical Chemistry A*, **2003**, 107, 6464-6469	2.8	28
20	Solvation of Yttrium with Ammonia: An Experimental and Theoretical Study. *Journal of Physical Chemistry A*, **2003**, 107, 9099-9104	2.8	7
19	Theoretical Study of the Structure and Bonding of a Metal□DNA Base Complex: Al□Guanine. *Journal of Physical Chemistry A*, **2003**, 107, 9415-9421	2.8	29
18	Interaction of Y, Y2, Mo, and Mo2 with NH3. A Density Functional Study. *Journal of Physical Chemistry A*, **2003**, 107, 4136-4140	2.8	4
17	Al3O4 and Al3O4- Clusters: Structure, Bonding, and Electron Binding Energies. *Journal of Physical Chemistry A*, **2003**, 107, 2589-2595	2.8	32
16	Al3On and Al3On- (n = 1□) Clusters: Structures, Photoelectron Spectra, Harmonic Vibrational Frequencies, and Atomic Charges. *Journal of Physical Chemistry A*, **2002**, 106, 10630-10635	2.8	47
15	INFRARED ASSIGNMENT OF BIS(GLYCOLATO)-BIS(PYRIDINE) METAL(II) COMPOUNDS AND CRYSTAL STRUCTURE OF TRANS-BIS(GLYCOLATO)-CIS-BIS(PYRIDINE)NICKEL(II) DIHYDRATE. *Journal of Coordination Chemistry*, **2001**, 54, 267-284	1.6	3
14	Electronic Structure of AlO2, AlO2-, Al3O5, and Al3O5- Clusters. *Journal of Physical Chemistry A*, **2001**, 105, 11291-11294	2.8	38
13	A density functional study of the reactivity and stability of mixed copper complexes. Is hardness the reason?. *Inorganic Chemistry*, **2001**, 40, 301-6	5.1	9
12	Electronic Structure of Al3On and Al3On- (n = 1□) Clusters. *Journal of Physical Chemistry A*, **2001**, 105, 8787-8793	2.8	45
11	Structure, Reactivity and Dynamics of Atomic and Molecular Clusters Using Density Functional Theory (DFT) and Other Tools. *Springer Series in Cluster Physics*, **1999**, 157-180		1
10	Molecular versus Dissociative Chemisorption of Nitric Oxide on Co2and Co3(Neutral and Cationic). A Density Functional Study. *Journal of Physical Chemistry A*, **1998**, 102, 4643-4651	2.8	12
9	Structure and properties of cobalt clusters up to the tetramer: A density-functional study. *Physical Review B*, **1997**, 55, 10905-10921	3.3	85
8	Reaction of a Mo Atom with H2, N2, and O2: A Density Functional Study. *Journal of Physical Chemistry A*, **1997**, 101, 1532-1541	2.8	20
7	The structure of triniobium dinitride from zero electron kinetic energy photoelectron spectroscopy and density functional calculations. *Chemical Physics Letters*, **1997**, 277, 71-78	2.5	25
6	Vibrational and geometric structures of Nb3C2 and Nb3C+2 from pulsed field ionization-zero electron kinetic energy photoelectron spectra and density functional calculations. *Journal of Chemical Physics*, **1996**, 105, 10663-10671	3.9	69
5	The structure of Nb3O and Nb3O+ determined by pulsed field ionization□zero electron kinetic energy photoelectron spectroscopy and density functional theory. *Journal of Chemical Physics*, **1995**, 103, 5335-5342	3.9	133

4	Aluminum clusters. A comparison between all electron and model core potential calculations. *Journal of Chemical Physics*, **1994**, 101, 10677-10685	3.9	34
3	Stability of charged aluminum clusters. *Physical Review B*, **1994**, 49, 17464-17467	3.3	21
2	Relationship between energy and hardness differences. *The Journal of Physical Chemistry*, **1993**, 97, 4059-4063		112
1	TDZD's: Selective and ATP Noncompetitive Glycogen Synthase Kinase 3 Inhibitors257-280		2