Enrique Cabaleiro-Lago

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/406116/publications.pdf

Version: 2024-02-01

112 papers	2,196 citations	218381 26 h-index	315357 38 g-index
113 all docs	113 docs citations	113 times ranked	2006 citing authors

#	Article	IF	Citations
1	Computational study of the dissociation of Hâ€“X acids (X=F,â€‰Cl,â€‰Br,â€‰I) in water clusters. Journal of Chemical Physics, 2002, 117, 3160-3168.	1.2	81
2	Analysis of the performance of DFT-D, M05-2X and M06-2X functionals for studying Ï€â‹¯Ï€ interactions. Chemical Physics Letters, 2013, 557, 170-175.	1.2	77
3	Criteria for the Elucidation of the Pseudopericyclic Character of the Cyclization of (Z)-1,2,4,6-Heptatetraene and Its Heterosubstituted Analogues: Magnetic Properties and Natural Bond Orbital Analysis. Chemistry - A European Journal, 2003, 9, 1837-1843.	1.7	66
4	DFT conformational study of cysteine in gas phase and aqueous solution. Computational and Theoretical Chemistry, 2000, 498, 191-200.	1.5	64
5	A Potential Function for Intermolecular Interaction in the Acetonitrile Dimer Constructed from ab Initio Data. Journal of Physical Chemistry A, 1997, 101, 8327-8334.	1.1	55
6	Computational Study on the Characteristics of the Interaction in NaphthaleneÂ·Â·Â·(H₂X)_{n=1,2} (X = O, S) Clusters. Journal of Physical Chemistry A, 2008, 112, 6344-6350.	1.1	54
7	Analytical Potentials for HF Dimer and Larger HF Clusters from ab Initio Calculations. Journal of Physical Chemistry A, 1998, 102, 2455-2465.	1.1	50
8	Substituted Corannulenes and Sumanenes as Fullerene Receptors. A Dispersion-Corrected Density Functional Theory Study. Journal of Physical Chemistry A, 2014, 118, 9521-9528.	1.1	49
9	A DFT study of substituent effects in corannulene dimers. Physical Chemistry Chemical Physics, 2011, 13, 21139.	1.3	48
10	Electrocyclization of (Z)-1,2,4,6-Heptatetraene and its Heterosubstituted Analogues: Pericyclic or Pseudopericyclic?. Angewandte Chemie - International Edition, 2002, 41, 1147-1150.	7.2	47
11	On the Nature of Ïƒâ€“Ïƒ, Ïƒâ€“Ï€, and Ï€â€“Ï€ Stacking in Extended Systems. ACS Omega, 2018, 3, 9348-9359.	1.6	46
12	Intermolecular interactions and cooperative effects in acetonitrile clusters. An ab initio molecular orbital study. Computational and Theoretical Chemistry, 2000, 498, 21-28.	1.5	45
13	DFT Study of the Interaction between Alkaline Cations and Molecular Bowls Derived from Fullerene. Journal of Physical Chemistry B, 2011, 115, 2774-2782.	1.2	45
14	A DFT Study of the Boultonâ^'Katritzky Rearrangement of (5R)-4-Nitrosobenz[c]isoxazole and Its Anion:â€‰Pseudopericyclic Reactions with Aromatic Transition States. Journal of Organic Chemistry, 2004, 69, 7013-7017.	1.7	41
15	Ab initio study of M(CH3CN)n clusters (M=Li+, Na+, Mg2+) in the gas phase. Chemical Physics, 2000, 254, 11-23.	0.9	40
16	DFT Study of Pericyclic and Pseudopericyclic Thermal Cheletropic Decarbonylations. Evaluation of Magnetic Properties. Journal of Organic Chemistry, 2003, 68, 8823-8830.	1.7	39
17	Influence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicals. Journal of Physical Chemistry A, 2018, 122, 4790-4800.	1.1	37
18	Ab initio study of interactions in methylamine clusters. The significance of cooperative effects. Journal of Chemical Physics, 2000, 112, 2155-2163.	1.2	36

#	Article	IF	Citations
19	Are Electrocyclization Reactions of (3Z)-1,3,5-Hexatrienone and Nitrogen Derivatives Pseudopericyclic? A DFT Study. Journal of Organic Chemistry, 2005, 70, 3921-3928.	1.7	34
20	Ab Initio Study of Interactions in Hydrazine Clusters of One To Four Molecules:â€‰ Cooperativity in the Interaction. Journal of Physical Chemistry A, 1999, 103, 6468-6474.	1.1	33
21	Theoretical characterization of structures and energies of benzeneâ€“(H2S)n and (H2S)n (n=1â€“4) clusters. Journal of Chemical Physics, 2005, 122, 204315.	1.2	33
22	Ring-annelated corannulenes as fullerene receptors. A DFT-D study. RSC Advances, 2014, 4, 29826-29833.	1.7	33
23	A Density Functional Theory Study of Rhodium-Catalyzed Hetero-[5+2]-cycloaddition of Cyclopropyl Imine Derivatives and Alkynes. Journal of Physical Chemistry A, 2008, 112, 9068-9074.	1.1	31
24	Study of the interaction between water and hydrogen sulfide with polycyclic aromatic hydrocarbons. Journal of Chemical Physics, 2009, 130, 234307.	1.2	28
25	The study of A(CH3OH)1â€“6 (A = Li+, Na+) in the gas phase based on ab initio calculations, analysis of the solvation process. Chemical Physics, 2000, 254, 109-123.	0.9	27
26	A Computational Study of Anion-Modulated Cationâˆ’Ï€ Interactions. Journal of Physical Chemistry B, 2012, 116, 5860-5871.	1.2	26
27	Fullerene recognition with molecular tweezers made up of efficient buckybowls: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2015, 17, 13206-13214.	1.3	26
28	Carbon-nanorings ([10]CPP and [6]CPPA) as fullerene (C60 and C70) receptors: a comprehensive dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2016, 18, 31670-31679.	1.3	26
29	Fullerene size controls the selective complexation of [11]CPP with pristine and endohedral fullerenes. Physical Chemistry Chemical Physics, 2018, 20, 11347-11358.	1.3	26
30	Cation-Ï€ and anion-Ï€ interactions: Changes in aromaticity upon complexation. Chemical Physics Letters, 2008, 452, 49-53.	1.2	25
31	A theoretical study of complexes between fullerenes and concave receptors with interest in photovoltaics. Physical Chemistry Chemical Physics, 2017, 19, 26787-26798.	1.3	25
32	Ab Initioand density functional theory study of the interaction in formamide and thioformamide dimers and trimers. Journal of Chemical Physics, 2002, 117, 1621-1632.	1.2	24
33	A Density Functional Theory Study on the Electrocyclization of 1,2,4,6-Heptatetraene Analogues: Converting a Pericyclic to a Pseudopericyclic Reaction. Chemistry - A European Journal, 2005, 11, 5966-5974.	1.7	24
34	Ab Initio and DFT Study of the Reaction Mechanism of Diformylketene with Formamide. Journal of Physical Chemistry A, 2004, 108, 8373-8377.	1.1	22
35	Interaction between anions and substituted molecular bowls. Physical Chemistry Chemical Physics, 2012, 14, 104-112.	1.3	22
36	Tailoring buckybowls for fullerene recognition. A dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2015, 17, 6233-6241.	1.3	22

#	Article	IF	Citations
37	Development of an intermolecular potential function for interactions in formamide clusters based on ab initio calculations. Journal of Chemical Physics, 1999, 110, 6782-6791.	1.2	20
38	Methanethiol Dimer and Trimer. An ab Initio and DFT Study of the Interaction. Journal of Physical Chemistry A, 2002, 106, 7440-7447.	1.1	20
39	Characteristics of the interaction of azulene with water and hydrogen sulfide: A computational study. Journal of Chemical Physics, 2008, 129, 084305.	1.2	20
40	On the mechanism of rhodium-catalyzed [6+2] cycloaddition of 2-vinylcyclobutanones and alkenes. Tetrahedron, 2008, 64, 6215-6220.	1.0	19
41	Water interaction with ion pairs from ionic liquids. Computational study and performance assessment of several common functionals. Chemical Physics Letters, 2014, 593, 181-188.	1.2	19
42	Evaluation of Magnetic Properties as a Criterion for the Elucidation of the Pseudopericyclic Character of 1,5-Electrocyclizations in Nitrile Ylides. Journal of Physical Chemistry A, 2003, 107, 4962-4966.	1.1	18
43	Ïƒâ€Ïƒ, Ïƒâ€Ï€, and Ï€â€Ï€ Stacking Interactions between Sixâ€Membered Cyclic Systems. Dispersion Dominates and Electrostatics Commands. ChemistrySelect, 2017, 2, 5157-5166.	0.7	18
44	An intermolecular potential function for Na+â€“acetonitrile obtained from ab initio calculations.. Chemical Physics, 1998, 236, 235-242.	0.9	17
45	Anab initiostudy of the interaction in dimethylamine dimer and trimer. Journal of Chemical Physics, 2000, 113, 9523-9531.	1.2	17
46	A DFT Study of the Concerted Cyclisation of 3-Azidopropenal to Isoxazole:Is it a Pseudopericyclic Reaction According to Its Magnetic Properties?. European Journal of Organic Chemistry, 2005, 2005, 3228-3232.	1.2	17
47	A DFT Study of the Pericyclic/Pseudopericyclic Character of Cycloaddition Reactions of Ethylene and Formaldehyde to Buta-1,3-dien-1-one and Derivatives. Journal of Physical Chemistry A, 2005, 109, 5636-5644.	1.1	17
48	Study of the ferroceneâ€“lithium cation interaction by DFT calculations: an in-depth analysis of the existence of a planetary system. Tetrahedron, 2009, 65, 2368-2371.	1.0	17
49	Effect of microhydration on the guanidiniumâ‹¯benzene interaction. Journal of Chemical Physics, 2011, 135, 214301.	1.2	17
50	Interaction between ions and substituted buckybowls: A comprehensive computational study. Journal of Computational Chemistry, 2014, 35, 1533-1544.	1.5	17
51	Endohedral alkali cations promote charge transfer transitions in complexes of C₆₀ with [10]cycloparaphenylenes. Physical Chemistry Chemical Physics, 2019, 21, 16665-16675.	1.3	17
52	Development of a potential function for describing the properties of HCN clusters. Journal of Chemical Physics, 1998, 108, 3598-3607.	1.2	16
53	Ab initio and DFT study of the aromaticity of some Fulvalenes derived from Methylidenecyclopropabenzene. Journal of Molecular Modeling, 2007, 13, 919-926.	0.8	16
54	A cooperative mechanism as the main source of the marked structural differences between solid and gaseous HCNâ‹¯BF3. Chemical Physics Letters, 1998, 294, 272-276.	1.2	15

#	Article	IF	Citations
55	Computational study of the dissociation of oxalic acid in water clusters. Chemical Physics, 2004, 302, 53-60.	0.9	15
56	Theoretical Study of the [2+2+2+1] Cycloaddition Mechanism of Enediynes and Carbon Monoxide Catalyzed by Rhodium. Journal of Physical Chemistry A, 2008, 112, 2423-2427.	1.1	15
57	Interaction of aromatic units of amino acids with guanidinium cation: The interplay of Ï€Â·Â·Â·Ï€, Xï£¿HÂ·Â·Â·Ï€, and M⁺Â·Â·Â·Ï€ contacts. Journal of Computational Chemistry, 2014, 35, 1290-1301.	1.5	15
58	A theoretical study of complexes formed between cations and curved aromatic systems: electrostatics does not always control cationâ€“Ï€ interaction. Physical Chemistry Chemical Physics, 2017, 19, 10543-10553.	1.3	15
59	Intermolecular potential for acetonitrile based onab initiocalculations. Molecular Physics, 1999, 96, 309-321.	0.8	14
60	A MP2 and DFT study of the aromatic character of polyphosphaphospholes. Is the pyramidality the only factor to take into consideration?. Journal of Molecular Modeling, 2011, 17, 1267-1272.	0.8	14
61	DFT and MP2 study of the interaction between corannulene and alkali cations. Journal of Molecular Modeling, 2013, 19, 2049-2055.	0.8	14
62	An ab Initio Study of M+(CH3OH)nClusters (M = K, Rb, Cs). Competition between Interior and Surface Structures. Journal of Physical Chemistry A, 2002, 106, 7195-7203.	1.1	13
63	A DFT study of the [4+2] cycloadditions of conjugated ketenes (vinylketene, imidoylketene and) Tj ETQq1 1 0.784314 rgBT /Overlock 1 properties. Tetrahedron, 2007, 63, 4937-4943.	1.0	13
64	On the interaction between the imidazolium cation and aromatic amino acids. A computational study. Organic and Biomolecular Chemistry, 2015, 13, 7961-7972.	1.5	13
65	Ab Initio and DFT Study of the Influence of the Allene Group on the Dielsâ€“Alder Reaction. Structural Chemistry, 2004, 15, 323-326.	1.0	12
66	A Comparative Theoretical Study of the Pericyclic-pseudopericyclic Character in a Group of Cyclizations of Dienylketenes to Cyclohexadienones. Journal of Physical Chemistry A, 2007, 111, 2935-2940.	1.1	12
67	Interaction of Anions with Substituted Buckybowls. The Anionâ€™s Nature and Solvent Effects. Journal of Physical Chemistry A, 2014, 118, 6112-6124.	1.1	12
68	Cationâ‹¯Ï€ interaction and microhydration effects in complexes formed by pyrrolidinium cation and aromatic species in amino acid side chains. Organic and Biomolecular Chemistry, 2014, 12, 2938.	1.5	12
69	Dissecting the concaveâ€“convex Ï€âˆ’Ï€ interaction in corannulene and sumanene dimers: SAPT(DFT) analysis and performance of DFT dispersionâ€corrected methods. Journal of Computational Chemistry, 2018, 39, 93-104.	1.5	12
70	Ab Initio MP2 and DFT Study of the Thermal Syn Elimination Reaction in Ethyl Formate. Journal of Physical Chemistry A, 2003, 107, 1651-1654.	1.1	11
71	Study of the interaction in clusters formed by phenol and CH3X (X=CN,F,Cl) molecules. Journal of Chemical Physics, 2008, 128, 194311.	1.2	11
72	A computational study of the mechanism of the unimolecular elimination of Î±,Î²-unsaturated aldehydes in the gas phase. Journal of Molecular Modeling, 2011, 17, 21-26.	0.8	11

#	Article	IF	Citations
73	A computational study of the protonation of simple amines in water clusters. Physical Chemistry Chemical Physics, 2013, 15, 18204.	1.3	11
74	An ab initio study of a model compound of penicillins. Computational and Theoretical Chemistry, 1999, 491, 177-185.	1.5	10
75	Computational Study of the Interaction in (CH3)2X Dimer and Trimer (X = O, S). Journal of Physical Chemistry A, 2004, 108, 4923-4929.	1.1	10
76	Theoretical study of the walk rearrangement in perfluorotetramethyl (Dewar thiophene) exo-S-oxide. Tetrahedron, 2007, 63, 2191-2198.	1.0	10
77	Computational study of the interaction of indole-like molecules with water and hydrogen sulfide. Journal of Chemical Physics, 2011, 135, 134310.	1.2	10
78	Synthesis and reactivity of thiosemicarbazone palladacycles. Crystal structure analysis and theoretical calculations. Inorganica Chimica Acta, 2016, 449, 20-30.	1.2	10
79	Potential functions for describing intermolecular interactions in cyanoacetylene clusters. Journal of Chemical Physics, 1998, 109, 8398-8406.	1.2	9
80	A quantum chemical study of aniline/ammonia clusters. Thermodynamic properties and frequency analysis. Computational and Theoretical Chemistry, 2000, 497, 105-113.	1.5	9
81	Study of the interaction between aniline and CH3CN, CH3Cl and CH3F. Theoretical Chemistry Accounts, 2011, 128, 531-539.	0.5	8
82	Effects of microhydration on the characteristics of cationâ€“phenol complexes. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	8
83	Effect of stepwise microhydration on the methylammoniumÂ·Â·Â·phenol and ammoniumÂ·Â·Â·phenol interaction. Journal of Molecular Modeling, 2013, 19, 1985-1994.	0.8	8
84	Interaction between the guanidinium cation and aromatic amino acids. Physical Chemistry Chemical Physics, 2014, 16, 22499-22512.	1.3	8
85	NCI analysis of the interaction cationâ‹¯Ï€ in complexes with molecular bowls derived from fullerene. Computational and Theoretical Chemistry, 2015, 1053, 123-129.	1.1	8
86	An ab initio study of the potential energy surface of methylamine dimer. Computational and Theoretical Chemistry, 2002, 586, 225-234.	1.5	7
87	A DFT Study of the Interaction between Microhydrated Anions and Naphthalendiimides. ChemPhysChem, 2012, 13, 570-577.	1.0	7
88	A computational study of the electrocyclization of o-divinylbenzene and derivatives. Computational and Theoretical Chemistry, 2007, 811, 141-151.	1.5	6
89	Density Functional Theory Study of Ruthenium (II)-Catalyzed [2+2+2] Cycloaddition of 1,6-Diynes with Tricarbonyl Compounds. Journal of Physical Chemistry A, 2008, 112, 8116-8120.	1.1	6
90	A theoretical study of ternary indoleâ€“cationâ€“anion complexes. Organic and Biomolecular Chemistry, 2014, 12, 9145-9156.	1.5	6

#	Article	IF	Citations
91	The relative position of Ï€â€“Ï€ interacting rings notably changes the nature of the substituent effect. Physical Chemistry Chemical Physics, 2020, 22, 12068-12081.	1.3	6
92	New Approach for Correcting Noncovalent Interactions in Semiempirical Quantum Mechanical Methods: The Importance of Multiple-Orientation Sampling. Journal of Chemical Theory and Computation, 2021, 17, 5556-5567.	2.3	6
93	A Potential Function for Describing Intermolecular Interactions in the Hydroxylamine Dimer. Journal of Physical Chemistry A, 1998, 102, 10358-10365.	1.1	5
94	Effect of stepwise microhydration on the guanidiniumÂ·Â·Â·Ï€ interaction. Journal of Molecular Modeling, 2014, 20, 2209.	0.8	5
95	A through-space description of substituent effects leads to inaccurate molecular electrostatic potentials and cationâÏ€ interactions in extended aromatic systems. Physical Chemistry Chemical Physics, 2016, 18, 13750-13753.	1.3	5
96	Assessment of electronic transitions involving intermolecular charge transfer in complexes formed by fullerenes and donorâ€“acceptor nanohoops. Physical Chemistry Chemical Physics, 2018, 20, 27791-27803.	1.3	5
97	Rational Design of Efficient Environmental Sensors: Ring-Shaped Nanostructures Can Capture Quat Herbicides. ACS Omega, 2018, 3, 16976-16988.	1.6	5
98	DFT Study of the Nucleophilic Addition of Water to Ketenes. European Journal of Organic Chemistry, 2007, 2007, 2344-2351.	1.2	4
99	A theoretical study of the influence of BF3 on the reaction path of the [4+2] cycloaddition of vinylketene with formaldimine. Tetrahedron, 2007, 63, 11617-11621.	1.0	4
100	An Alternative Mechanism to Explain the Ruthenium(II)-Catalyzed [2 + 2 + 2] Cycloaddition of 1,6-Diynes and Tricarbonyl Compounds. Journal of Physical Chemistry A, 2009, 113, 9180-9184.	1.1	4
101	Comment on â€œTheoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamicsâ€• by H. Isobe, K. Nakamura, S. Hitosugi, S. Sato, H. Tokoyama, H. Yamakado, K. Ohno and H. Kono, Chem. Sci., 2015, 6, 2746. Chemical Science, 2016, 7, 2924-2928.	3.7	4
102	Curvature and size effects hinder halogen bonds with extended Ï€ systems. Physical Chemistry Chemical Physics, 2020, 22, 21988-22002.	1.3	4
103	Electrostatic penetration effects stand at the heart of aromatic Ï€ interactions. Physical Chemistry Chemical Physics, 2022, 24, 8979-8991.	1.3	4
104	Comment on â€œA Theoretical Investigation of the Interactions between Water Molecules and Ionic Liquidsâ€• Journal of Physical Chemistry B, 2008, 112, 13465-13466.	1.2	3
105	A DFT study of a model compound of vitamin D. Computational and Theoretical Chemistry, 1999, 492, 143-150.	1.5	2
106	A Theoretical Study of Pericyclic Rearrangements Catalyzed by Lithium. Journal of Physical Chemistry A, 2008, 112, 5218-5223.	1.1	2
107	A MP2 and DFT study of the influence of complexation on the aromatic character of phosphole. Journal of Molecular Modeling, 2012, 18, 765-770.	0.8	2
108	Size and shape effects on complexes of fullerenes with carbon nanorings: C50 and C76 as [10]CPP and [6]CPPA guests. Structural Chemistry, 2019, 30, 647-656.	1.0	2

#	Article	IF	Citations
109	The PM6-FGC Method: Improved Corrections for Amines and Amides. Molecules, 2022, 27, 1678.	1.7	2
110	Computational Study of the Interaction in X-(CH3NH2)n Clusters (X = F, Cl; n = 1â^'4). The Balance between Ionâ^'Molecule and Moleculeâ^'Molecule Interactions. Journal of Physical Chemistry A, 2003, 107, 10184-10190.	1.1	1
111	Intermolecular potential for acetonitrile based on ab initio calculations. , 0, .		1
112	Theoretical study of the decomposition of ethyl and ethyl 3-phenyl glycidate. Journal of Molecular Modeling, 2013, 19, 315-320.	0.8	0