AdriÃ Gil

List of Publications by Year
in descending order

47 papers	1,304 citations	394421 19 h-index	345221 36 g-index
51 all docs	51 docs citations	51 times ranked	1825 citing authors

#	Article	IF	Citations
1	Semi-empirical and linear-scaling DFT methods to characterize duplex DNA and G-quadruplexes in the presence of interacting small molecules. Physical Chemistry Chemical Physics, 2022, 24, 11510-11519.	2.8	5
2	Influence of conventional hydrogen bonds in the intercalation of phenanthroline derivatives with DNA: The important role of the sugar and phosphate backbone. Journal of Computational Chemistry, 2022, 43, 804-821.	3.3	5
3	Computational Modelling of the Interactions Between Polyoxometalates and Biological Systems. Frontiers in Chemistry, 2022, 10, 876630.	3.6	9
4	Greener Strategy for Lupanine Purification from Lupin Bean Wastewaters Using a Molecularly Imprinted Polymer. ACS Applied Materials & Interfaces, 2022, , .	8.0	2
5	Elucidating the intercalation of methylated 1,10-phenanthroline with DNA: the important weight of the CH/H interactions and the selectivity of CH/Ï€ and CH/n interactions. RSC Advances, 2021, 11, 1553-1563.	3.6	9
6	Electron-Transfer-Induced Side-Chain Cleavage in Tryptophan Facilitated through Potassium-Induced Transition-State Stabilization in the Gas Phase. Journal of Physical Chemistry A, 2021, 125, 2324-2333.	2.5	3
7	Learning to Model G-Quadruplexes: Current Methods and Perspectives. Annual Review of Biophysics, 2021, 50, 209-243.	10.0	21
8	Probing the Catalytically Active Species in POMâ€Catalysed DNAâ€Model Hydrolysis**. Chemistry - A European Journal, 2021, 27, 8977-8984.	3.3	7
9	Mechanistic Insights into Promoted Hydrolysis of Phosphoester Bonds by MoO2Cl2(DMF)2. Inorganic Chemistry, 2021, 60, 11177-11191.	4.0	5
10	New Insights on the Interaction of Phenanthroline Based Ligands and Metal Complexes and Polyoxometalates with Duplex DNA and G-Quadruplexes. Molecules, 2021, 26, 4737.	3.8	21
11	Photocatalytic degradation of acetaminophen and caffeine using magnetiteâ€“hematite combined nanoparticles: kinetics and mechanisms. Environmental Science and Pollution Research, 2021, 28, 17228-17243.	5.3	15
12	From Groove Binding to Intercalation: Unravelling the Weak Interactions and Other Factors Modulating the Modes of Interaction between Methylated Phenanthroline Based Drugs and Duplex DNA. Physical Chemistry Chemical Physics, 2021, 23, 26680-26695.	2.8	4
13	Computational Studies on the Binding Preferences of Molybdenum(II) Phenanthroline Complexes with Duplex DNA. The Important Role of the Ancillary Ligands. Inorganic Chemistry, 2020, 59, 12711-12721.	4.0	15
14	Unraveling the Modulation of the Activity in Drugs Based on Methylated Phenanthroline When Intercalating between DNA Base Pairs. Journal of Chemical Information and Modeling, 2019, 59, 3989-3995.	5.4	12
15	A model of tetrahydrofuran low-temperature oxidation based on theoretically calculated rate constants. Combustion and Flame, 2018, 191, 252-269.	5.2	36
16	On the H₂ interactions with transition metal adatoms supported on graphene: a systematic density functional study. Physical Chemistry Chemical Physics, 2018, 20, 3819-3830.	2.8	22
17	Electrochemical studies and potential anticancer activity in ferrocene derivatives. Journal of Coordination Chemistry, 2017, 70, 314-327.	2.2	22
18	Unravelling the dissociation pathways of acetic acid upon electron transfer in potassium collisions: experimental and theoretical studies. Physical Chemistry Chemical Physics, 2017, 19, 1083-1088.	2.8	5

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19	Effects of oxygenation on the intercalation of 1,10-phenanthroline-5,6/4,7-dione between DNA base pairs: a computational study. Physical Chemistry Chemical Physics, 2017, 19, 16638-16649.	2.8	18
20	Selfâ€Assembly of Uranylâ€“Peroxide Nanocapsules in Basic Peroxidic Environments. Chemistry - A European Journal, 2016, 22, 8571-8578.	3.3	32
21	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.	7.4	4
22	A theoretical study of methylation and CH/Ï€ interactions in DNA intercalation: methylated 1,10-phenanthroline in adenineâ€“thymine base pairs. RSC Advances, 2016, 6, 85891-85902.	3.6	23
23	Complex internal rearrangement processes triggered by electron transfer to acetic acid. Journal of Physics: Conference Series, 2015, 635, 012002.	0.4	0
24	Trends in the Hydrogen Activation and Storage by Adsorbed 3d Transition Metal Atoms onto Graphene and Nanotube Surfaces: A DFT Study and Molecular Orbital Analysis. Journal of Physical Chemistry C, 2015, 119, 5506-5522.	3.1	59
25	Synthesis and reactivity of TADDOL-based chiral Fe(<scp>ii</scp>) PNP pincer complexes-solution equilibria between Îº²P,N- and Îº³P,N,P-bound PNP pincer ligands. Dalton Transactions, 2015, 44, 13071-13086.	3.3	13
26	How the Intercalation of Phenanthroline Affects the Structure, Energetics, and Bond Properties of DNA Base Pairs: Theoretical Study Applied to Adenineâ€“Thymine and Guanineâ€“Cytosine Tetramers. Journal of Chemical Theory and Computation, 2015, 11, 2714-2728.	5.3	28
27	The Energy Landscape of Uranylâ€“Peroxide Species. Chemistry - A European Journal, 2014, 20, 3646-3651.	3.3	22
28	Six-coordinate high-spin iron(<scp>ii</scp>) complexes with bidentate PN ligands based on 2-aminopyridine â€“ new Fe(<scp>ii</scp>) spin crossover systems. Dalton Transactions, 2014, 43, 11152-11164.	3.3	15
29	Four- and five-coordinate high-spin iron(II) complexes bearing bidentate soft/hard SN ligands based on 2-aminopyridine. Polyhedron, 2014, 81, 45-55.	2.2	5
30	Catalysis in a Porous Molecular Capsule: Activation by Regulated Access to Sixty Metal Centers Spanning a Truncated Icosahedron. Journal of the American Chemical Society, 2012, 134, 13082-13088.	13.7	81
31	A Journey inside the U₂₈ Nanocapsule. Chemistry - A European Journal, 2012, 18, 8340-8346.	3.3	39
32	Modulation of Lipidâ€Induced ER Stress by Fatty Acid Shape. Traffic, 2011, 12, 349-362.	2.7	72
33	Novel triazolyl derivatives for acidic release of amines. Tetrahedron, 2011, 67, 401-407.	1.9	7
34	Trends in the Adsorption of 3d Transition Metal Atoms onto Graphene and Nanotube Surfaces: A DFT Study and Molecular Orbital Analysis. Journal of Physical Chemistry C, 2010, 114, 14141-14153.	3.1	184
35	On the Origin of the Cation Templated Self-Assembly of Uranyl-Peroxide Nanoclusters. Journal of the American Chemical Society, 2010, 132, 17787-17794.	13.7	102
36	Influence of ionization on the conformational preferences of peptide models. Ramachandran surfaces of Nâ€formylâ€glycine amide and Nâ€formylâ€alanine amide radical cations. Journal of Computational Chemistry, 2009, 30, 1771-1784.	3.3	8

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37	An Analysis of the Different Behavior of DNA and RNA through the Study of the Mutual Relationship between Stacking and Hydrogen Bonding. Journal of Physical Chemistry B, 2009, 113, 4907-4914.	2.6	47
38	How the site of ionisation influences side-chain fragmentation in histidine radical cation. Chemical Physics Letters, 2008, 451, 276-281.	2.6	14
39	Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. Journal of Chemical Theory and Computation, 2007, 3, 2210-2220.	5.3	41
40	CH/Ï€ Interactions in DNA and Proteins. A Theoretical Study. Journal of Physical Chemistry B, 2007, 111, 9372-9379.	2.6	55
41	Base-Catalyzed Anti-Markovnikov Hydroamination of Vinylarenes â€“ Scope, Limitations and Computational Studies. European Journal of Organic Chemistry, 2007, 2007, 3311-3325.	2.4	84
42	Gas-phase proton-transport self-catalysed isomerisation of glutamine radical cation: The important role of the side-chain. Theoretical Chemistry Accounts, 2007, 118, 589-595.	1.4	9
43	Effects of ionization on N-glycylglycine peptide: Influence of intramolecular hydrogen bonds. Journal of Chemical Physics, 2006, 124, 154306.	3.0	26
44	Structure and fragmentation of glycine, alanine, serine and cysteine radical cations. A theoretical study. Computational and Theoretical Chemistry, 2005, 727, 191-197.	1.5	63
45	Unusual hydrogen bonds in [AH3â€“H3O]+ radical cations (A=C, Si, Ge, Sn and Pb). Chemical Physics Letters, 2004, 395, 27-32.	2.6	4
46	Unusual hydrogen bonds in [AH3â€“H3O]+ radical cations (A=C, Si, Ge, Sn and Pb)Single-electron hydrogen bond, proton-hydride hydrogen bond and formation of [H2AOH2]+â€“H2 complexes. Chemical Physics Letters, 2004, 395, 27-32.	2.6	12
47	Gas Phase Dissociation Energies of Saturated AHnÂ·+Radical Cations and AHnNeutrals (A = Liâ^'F, Naâ^'Cl):Â Dehydrogenation, Deprotonation, and Formation of AHn-2Â·+ÂÂ â^' H2Complexes. Journal of the American Chemical Society, 2003, 125, 7461-7469.	13.7	18