

Adriã Gil

List of Publications by Year in descending order

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47
papers

1,304
citations

394421

19
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345221

36
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docs citations

51
times ranked

1825
citing authors

#	ARTICLE	IF	CITATIONS
1	Trends in the Adsorption of 3d Transition Metal Atoms onto Graphene and Nanotube Surfaces: A DFT Study and Molecular Orbital Analysis. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14141-14153.	3.1	184
2	On the Origin of the Cation Templated Self-Assembly of Uranyl-Peroxide Nanoclusters. <i>Journal of the American Chemical Society</i> , 2010, 132, 17787-17794.	13.7	102
3	Base-Catalyzed Anti-Markovnikov Hydroamination of Vinylarenes â€“ Scope, Limitations and Computational Studies. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 3311-3325.	2.4	84
4	Catalysis in a Porous Molecular Capsule: Activation by Regulated Access to Sixty Metal Centers Spanning a Truncated Icosahedron. <i>Journal of the American Chemical Society</i> , 2012, 134, 13082-13088.	13.7	81
5	Modulation of Lipidâ€“Induced ER Stress by Fatty Acid Shape. <i>Traffic</i> , 2011, 12, 349-362.	2.7	72
6	Structure and fragmentation of glycine, alanine, serine and cysteine radical cations. A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2005, 727, 191-197.	1.5	63
7	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. <i>Journal of Physical Chemistry C</i> , 2015, 119, 5506-5522.	3.1	59
8	CH/Ï€ Interactions in DNA and Proteins. A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9372-9379.	2.6	55
9	An Analysis of the Different Behavior of DNA and RNA through the Study of the Mutual Relationship between Stacking and Hydrogen Bonding. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4907-4914.	2.6	47
10	Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2210-2220.	5.3	41
11	A Journey inside the U ₂₈ Nanocapsule. <i>Chemistry - A European Journal</i> , 2012, 18, 8340-8346.	3.3	39
12	A model of tetrahydrofuran low-temperature oxidation based on theoretically calculated rate constants. <i>Combustion and Flame</i> , 2018, 191, 252-269.	5.2	36
13	Self-Assembly of Uranylâ€“Peroxide Nanocapsules in Basic Peroxidic Environments. <i>Chemistry - A European Journal</i> , 2016, 22, 8571-8578.	3.3	32
14	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. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2714-2728.	5.3	28
15	Effects of ionization on N-glycylglycine peptide: Influence of intramolecular hydrogen bonds. <i>Journal of Chemical Physics</i> , 2006, 124, 154306.	3.0	26
16	A theoretical study of methylation and CH/Ï€ interactions in DNA intercalation: methylated 1,10-phenanthroline in adenineâ€“thymine base pairs. <i>RSC Advances</i> , 2016, 6, 85891-85902.	3.6	23
17	The Energy Landscape of Uranylâ€“Peroxide Species. <i>Chemistry - A European Journal</i> , 2014, 20, 3646-3651.	3.3	22
18	Electrochemical studies and potential anticancer activity in ferrocene derivatives. <i>Journal of Coordination Chemistry</i> , 2017, 70, 314-327.	2.2	22

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19	On the H ₂ interactions with transition metal adatoms supported on graphene: a systematic density functional study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3819-3830.	2.8	22
20	Learning to Model G-Quadruplexes: Current Methods and Perspectives. <i>Annual Review of Biophysics</i> , 2021, 50, 209-243.	10.0	21
21	New Insights on the Interaction of Phenanthroline Based Ligands and Metal Complexes and Polyoxometalates with Duplex DNA and G-Quadruplexes. <i>Molecules</i> , 2021, 26, 4737.	3.8	21
22	Gas Phase Dissociation Energies of Saturated AHn ⁺ Radical Cations and AHnNeutrals (A = Li ⁺ , Na ⁺ , Cl ⁻): ⁺ Dehydrogenation, Deprotonation, and Formation of AHn-2 ⁺ H ₂ Complexes. <i>Journal of the American Chemical Society</i> , 2003, 125, 7461-7469.	13.7	18
23	Effects of oxygenation on the intercalation of 1,10-phenanthroline-5,6,4,7-dione between DNA base pairs: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16638-16649.	2.8	18
24	Six-coordinate high-spin iron(II) complexes with bidentate PN ligands based on 2-aminopyridine – new Fe(II) spin crossover systems. <i>Dalton Transactions</i> , 2014, 43, 11152-11164.	3.3	15
25	Computational Studies on the Binding Preferences of Molybdenum(II) Phenanthroline Complexes with Duplex DNA. The Important Role of the Ancillary Ligands. <i>Inorganic Chemistry</i> , 2020, 59, 12711-12721.	4.0	15
26	Photocatalytic degradation of acetaminophen and caffeine using magnetite-hematite combined nanoparticles: kinetics and mechanisms. <i>Environmental Science and Pollution Research</i> , 2021, 28, 17228-17243.	5.3	15
27	How the site of ionisation influences side-chain fragmentation in histidine radical cation. <i>Chemical Physics Letters</i> , 2008, 451, 276-281.	2.6	14
28	Synthesis and reactivity of TADDOL-based chiral Fe(II) PNP pincer complexes-solution equilibria between ² P,N- and ³ P,N,P-bound PNP pincer ligands. <i>Dalton Transactions</i> , 2015, 44, 13071-13086.	3.3	13
29	Unusual hydrogen bonds in [AH ₃ +H ₃ O] ⁺ radical cations (A=C, Si, Ge, Sn and Pb)Single-electron hydrogen bond, proton-hydride hydrogen bond and formation of [H ₂ AOH ₂] ⁺ H ₂ complexes. <i>Chemical Physics Letters</i> , 2004, 395, 27-32.	2.6	12
30	Unraveling the Modulation of the Activity in Drugs Based on Methylated Phenanthroline When Intercalating between DNA Base Pairs. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3989-3995.	5.4	12
31	Gas-phase proton-transport self-catalysed isomerisation of glutamine radical cation: The important role of the side-chain. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 589-595.	1.4	9
32	Elucidating the intercalation of methylated 1,10-phenanthroline with DNA: the important weight of the CH/H and CH/n interactions and the selectivity of CH/H and CH/n interactions. <i>RSC Advances</i> , 2021, 11, 1553-1563.	3.6	9
33	Computational Modelling of the Interactions Between Polyoxometalates and Biological Systems. <i>Frontiers in Chemistry</i> , 2022, 10, 876630.	3.6	9
34	Influence of ionization on the conformational preferences of peptide models. Ramachandran surfaces of <i>N</i> -formylglycine amide and <i>N</i> -formylalanine amide radical cations. <i>Journal of Computational Chemistry</i> , 2009, 30, 1771-1784.	3.3	8
35	Novel triazolyl derivatives for acidic release of amines. <i>Tetrahedron</i> , 2011, 67, 401-407.	1.9	7
36	Probing the Catalytically Active Species in POM-Catalysed DNA-Model Hydrolysis**. <i>Chemistry - A European Journal</i> , 2021, 27, 8977-8984.	3.3	7

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37	Four- and five-coordinate high-spin iron(II) complexes bearing bidentate soft/hard SN ligands based on 2-aminopyridine. <i>Polyhedron</i> , 2014, 81, 45-55.	2.2	5
38	Unravelling the dissociation pathways of acetic acid upon electron transfer in potassium collisions: experimental and theoretical studies. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1083-1088.	2.8	5
39	Mechanistic Insights into Promoted Hydrolysis of Phosphoester Bonds by MoO ₂ Cl ₂ (DMF) ₂ . <i>Inorganic Chemistry</i> , 2021, 60, 11177-11191.	4.0	5
40	Semi-empirical and linear-scaling DFT methods to characterize duplex DNA and G-quadruplexes in the presence of interacting small molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11510-11519.	2.8	5
41	Influence of conventional hydrogen bonds in the intercalation of phenanthroline derivatives with DNA: The important role of the sugar and phosphate backbone. <i>Journal of Computational Chemistry</i> , 2022, 43, 804-821.	3.3	5
42	Unusual hydrogen bonds in [AH ₃ â€“H ₃ O] ⁺ radical cations (A=C, Si, Ge, Sn and Pb). <i>Chemical Physics Letters</i> , 2004, 395, 27-32.	2.6	4
43	Comment on “Theoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamics” by H. Isobe, K. Nakamura, S. Hitosugi, S. Sato, H. Tokoyama, H. Yamakado, K. Ohno and H. Kono, <i>Chem. Sci.</i> , 2015, 6, 2746. <i>Chemical Science</i> , 2016, 7, 2924-2928.	7.4	4
44	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. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26680-26695.	2.8	4
45	Electron-Transfer-Induced Side-Chain Cleavage in Tryptophan Facilitated through Potassium-Induced Transition-State Stabilization in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2324-2333.	2.5	3
46	Greener Strategy for Lupanine Purification from Lupin Bean Wastewaters Using a Molecularly Imprinted Polymer. <i>ACS Applied Materials & Interfaces</i> , 2022, , .	8.0	2
47	Complex internal rearrangement processes triggered by electron transfer to acetic acid. <i>Journal of Physics: Conference Series</i> , 2015, 635, 012002.	0.4	0