JosÃ©-Manuel M MartÃ-nez-MagadÃ¡n

List of Publications by Year
in descending order

73	1,437	331642	377849
papers	citations	21 h-index	34 g-index

77	77	77	1557
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Critical micelle concentration of SDS through DPD simulations using COSMO-RSâ€“based interaction parameters, the thermal effects. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 645, 128867.	4.7	8
2	Foaming supramolecular surfactants for gas mobility control in naturally fractured carbonate reservoirs at high temperature, salinity, and hardness. Petroleum Science, 2022, 19, 3134-3148.	4.9	6
3	Quantum modeling design of imidazoline-based corrosion inhibitors for oil industry applications. Materials Today Communications, 2021, 27, 102466.	1.9	4
4	Development through computational design of a new terpolymer with anti-scale properties applied to the oil production assurance process. Fuel, 2020, 282, 118832.	6.4	3
5	Synthesis and Photocatalytic Activity of Cu2O Microspheres upon Methyl Orange Degradation. Topics in Catalysis, 2020, 63, 586-600.	2.8	14
6	Density Functional Theory and UPLC/MS/ESI+ studies of the zwitterionic surfactant-Na+ pair formation. Journal of Molecular Graphics and Modelling, 2019, 91, 204-213.	2.4	2
7	H₂ Solubility in Hydrocarbons Calculated by the COSMO-RS Method. Industrial & Engineering Chemistry Research, 2019, 58, 12361-12368.	3.7	4
8	Quantum molecular design and experimental testing of a high-performance zwitterionic corrosion inhibitor for oxidized iron surfaces. Journal of Molecular Graphics and Modelling, 2019, 93, 107444.	2.4	3
9	A theoretical study of crude oil emulsions stability due to supramolecular assemblies. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2019, 567, 121-127.	4.7	14
10	Molecular modeling, synthesis and characterization of branched geminal zwitterionic liquids for enhanced oil recovery. Arabian Journal of Chemistry, 2019, 12, 4212-4219.	4.9	7
11	Solid and liquid supramolecular complexes by solid-solid mechanosynthesis. Arabian Journal of Chemistry, 2019, 12, 4664-4674.	4.9	1
12	Molecular design of high performance zwitterionic liquids for enhanced heavy-oil recovery processes. Journal of Molecular Graphics and Modelling, 2018, 80, 264-271.	2.4	7
13	Nonquilibrium and Equilibrium Stationary States of Zwitterionic Surfactant Dynamic Adsorption on Limestone Cores at Oil-Reservoir Conditions. Industrial & Engineering Chemistry Research, 2018, 57, 2075-2082.	3.7	6
14	Deep oxidative desulfurization with simultaneous oxidative denitrogenation of diesel fuel and straight run gas oil. Applied Catalysis B: Environmental, 2018, 236, 326-337.	20.2	68
15	Experimental and Theoretical Study on Supramolecular Ionic Liquid (IL)â€“Asphaltene Complex Interactions and Their Effects on the Flow Properties of Heavy Crude Oils. Journal of Physical Chemistry B, 2018, 122, 4325-4335.	2.6	17
16	Calculation of the Solubility Parameter by COSMO-RS Methods and Its Influence on Asphalteneâ€“Ionic Liquid Interactions. Industrial & Engineering Chemistry Research, 2017, 56, 5107-5115.	3.7	24
17	Green-Inspired Synthesis and Industrial Applications of Branched Geminal Zwitterionic Liquids. ACS Sustainable Chemistry and Engineering, 2017, 5, 6404-6408.	6.7	1
18	Synthesis of branched geminal zwitterionic liquids as wettability modifiers in enhanced oil recovery processes. Journal of Industrial and Engineering Chemistry, 2017, 45, 44-55.	5.8	17

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19	Theoretical Study of the Aliphatic-Chain Lengthâ€™s Electronic Effect on the Corrosion Inhibition Activity of Methylimidazole-Based Ionic Liquids. Industrial & Engineering Chemistry Research, 2016, 55, 3506-3516.	3.7	33
20	Behavior of ionic species in sulfonated PEI using DFT simulations: A study to determine ionic conductivity. International Journal of Hydrogen Energy, 2015, 40, 17332-17337.	7.1	4
21	Supramolecular pairing among heteroaromatic compounds and the cationic surfactant C12TAC. Fuel, 2015, 149, 174-183.	6.4	8
22	Theoretical and experimental insights into the control of calcium sulfate scales by using random copolymers based on itaconic acid. Fuel, 2015, 149, 66-77.	6.4	21
23	Role of sulfonation in the stability, reactivity, and selectivity of poly(ether imide) used to develop ion exchange membranes: DFT study with application to fuel cells. Journal of Molecular Modeling, 2014, 20, 2325.	1.8	8
24	Theoretical and experimental insights on the true impact of C12TAC cationic surfactant in enhanced oil recovery for heavy oil carbonate reservoirs. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2014, 455, 76-91.	4.7	31
25	Quantum chemical characterization of zwitterionic structures: Supramolecular complexes for modifying the wettability of oilâ€“waterâ€“limestone system. Journal of Molecular Graphics and Modelling, 2014, 51, 128-136.	2.4	15
26	N-aryl amino-alcohols as stabilizers of asphaltenes. Fuel, 2013, 110, 302-309.	6.4	30
27	Critical micelle concentration of an ammonium salt through DPD simulations using COSMOâ€RSâ€“based interaction parameters. AICHE Journal, 2013, 59, 4413-4423.	3.6	14
28	Electrochemistry, Reactivity and Selectivity of Toroidal C₁₂₀ Nanostructure: A Density Functional Theory Study. Journal of Computational and Theoretical Nanoscience, 2012, 9, 1014-1022.	0.4	2
29	Density Functional Theoretical Study of the Interaction of Geminal Zwitterionic Liquids with Limestone, Regarding the Behavior of the Wettability Parameter. Journal of Chemical & Engineering Data, 2012, 57, 3538-3542.	1.9	11
30	DFT study of the interaction between ethanethiol and Fe-containing ionic liquids for desulfuration of natural gasoline. Fuel Processing Technology, 2012, 97, 24-29.	7.2	49
31	DFT Study of the CO Poisoning Effects on Pd_xCu_{1-x} (110) Surface. Journal of New Materials for Electrochemical Systems, 2012, 15, 151-156.	0.6	0
32	Vibrational analysis and thermodynamic properties of C120 nanotorus: a DFT study. Journal of Nanoparticle Research, 2011, 13, 6649-6659.	1.9	5
33	Theoretical studies of ionic conductivity of crosslinked chitosan membranes. International Journal of Hydrogen Energy, 2010, 35, 12141-12146.	7.1	42
34	A DFT study of the electronic structure of cobalt and nickel mono-substituted MoS2 triangular nanosized clusters. Journal of Molecular Catalysis A, 2009, 313, 49-54.	4.8	14
35	Mesoscopic study of cylindrical phases of poly(styrene)-poly(isoprene) copolymer: Orderâ€“order phase transitions by temperature control. Polymer, 2009, 50, 4596-4601.	3.8	10
36	Mesoscopic simulation of metastable microphases in the orderâ€“order transition from gyroid-to-lamellar states of PSâ€“PI diblock copolymer. Chemical Physics Letters, 2008, 460, 507-511.	2.6	11

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37	Proton affinity of S-containing aromatic compounds: Implications for crude oil hydrodesulfurization. Journal of Molecular Catalysis A, 2008, 281, 79-84.	4.8	32
38	Dissipative Particle Dynamics Study of Orderâ^'Order Phase Transition of BCC, HPC, OBDD, and LAM Structures of the Poly(styrene)â^'Poly(isoprene) Diblock Copolymer. Macromolecules, 2008, 41, 3297-3304.	4.8	55
39	Methodology for Predicting the Phase Envelope of a Heavy Crude Oil and Its Asphaltene Deposition Onset. Petroleum Science and Technology, 2007, 25, 19-39.	1.5	10
40	DFT Molecular Dynamics Study of Pyrene Biradical Species. Petroleum Science and Technology, 2007, 25, 67-80.	1.5	4
41	Molecular Characterization ofp-Alkyl Phenolâ^'n-Heptane Interactions and Their Implication as Asphaltene Dispersants. Energy & Fuels, 2007, 21, 1127-1132.	5.1	14
42	Self-Organization Process of Ordered Structures in Linear and Star Poly(styrene)â^'Poly(isoprene) Block Copolymers:â€‰ Gaussian Models and Mesoscopic Parameters of Polymeric Systems. Journal of Physical Chemistry B, 2007, 111, 11756-11764.	2.6	46
43	Mesoscopic simulation of asymmetric-copolymer/homopolymer blends: Microphase morphological modification by homopolymer chains solubilization. Polymer, 2007, 48, 3902-3911.	3.8	23
44	Correlation between Electronic Properties and Hydrodesulfurization Activity of 4d-Transition-Metal Sulfides. Journal of Physical Chemistry B, 2006, 110, 7951-7966.	2.6	25
45	Application of molecular simulation to calculate miscibility of a model asphaltene molecule. Fluid Phase Equilibria, 2006, 239, 100-106.	2.5	43
46	Theoretical study of nickel porphyrinate derivatives related to catalyst dopant in the oil industry. Journal of Molecular Catalysis A, 2005, 228, 195-202.	4.8	5
47	Molecular modeling and simulation of ion-conductivity in chitosan membranes. Polymer, 2005, 46, 7519-7527.	3.8	36
48	Molecular simulation of diblock copolymers; morphology and mechanical properties. Polymer, 2005, 46, 7485-7493.	3.8	36
49	DFTâ€"Quantum chemical study of the HZSM-5-cyclohexene interaction pathways. Journal of Molecular Catalysis A, 2005, 236, 194-205.	4.8	3
50	Cracking of n-heptane in HZSM-5 zeolite. Computational and Theoretical Chemistry, 2005, 755, 99-103.	1.5	4
51	Topological analysis of the electron density and of the electron localization function of pyrene and its radicals. Chemical Physics, 2005, 308, 181-192.	1.9	21
52	Electronic Structure Properties of Dibenzofurane and Dibenzothiophene Derivatives:â€‰ Implications on Asphaltene Formation. Energy & Fuels, 2005, 19, 998-1002.	5.1	11
53	A Theoretical Study of Dibenzothiophene Absorbed on Open-Ended Carbon Nanotubes. Journal of Physical Chemistry B, 2005, 109, 14868-14875.	2.6	25
54	Theoretical Study of a New Group of Corrosion Inhibitors. Journal of Physical Chemistry A, 2005, 109, 8950-8957.	2.5	72

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55	On the geometric structure of the (0001) hematite surface. Surface Science, 2004, 558, 4-14.	1.9	48
56	Effect of Ni and Co impurities on the electronic structure and magnetic properties of BCC iron. Journal of Magnetism and Magnetic Materials, 2004, 280, 293-303.	2.3	1
57	Docking of An Asphaltene Molecular Model on A Fe2O3Surface, An Ab Initio Simulated Annealing. Petroleum Science and Technology, 2004, 22, 915-926.	1.5	11
58	Morphology of Aggregated Asphaltene Structural Models. Energy & Fuels, 2004, 18, 1676-1686.	5.1	92
59	Theoretical Prediction of Benzyne-Like Species in Pyrene Diradicals. Journal of Physical Chemistry A, 2004, 108, 5111-5116.	2.5	16
60	Preliminary Study of the Effect of Pressure on Asphaltene Disassociation by Molecular Dynamics. Petroleum Science and Technology, 2004, 22, 927-942.	1.5	19
61	Electronic structure in different environments for vanadyl porphyrinate molecules present in crude oil. Computational and Theoretical Chemistry, 2003, 626, 195-201.	1.5	15
62	Asphaltene Aggregation under Vacuum at Different Temperatures by Molecular Dynamics. Energy & Fuels, 2003, 17, 1346-1355.	5.1	127
63	Electronic Structure Properties of Carbazole-like Compounds:Â Implications for Asphaltene Formation. Journal of Physical Chemistry A, 2003, 107, 1597-1603.	2.5	16
64	An embedded QM/MM study for different SiO2/Al2O3ratios of the HZSM-5 zeolite and for their interaction with n-heptane. International Journal of Quantum Chemistry, 2002, 88, 750-766.	2.0	12
65	A comparative DFT study of the catalytic activity of the 3d transition metal sulphides surfaces. Surface Science, 2002, 518, 163-173.	1.9	12
66	Theoretical study of high-valent vanadium oxo-porphyrins as a dopant of crude oil. Computational and Theoretical Chemistry, 2001, 542, 115-121.	1.5	6
67	DFT study of the interaction of the HZSM-5 zeolite with the benzene molecule. International Journal of Quantum Chemistry, 2000, 80, 125-132.	2.0	16
68	Promotional effect of Co or Ni impurity in the catalytic activity of MoS2: An electronic structure study. International Journal of Quantum Chemistry, 2000, 80, 406-415.	2.0	5
69	Theoretical study for the Pt2Au- and PtAu2- ethylene interaction. International Journal of Quantum Chemistry, 1999, 75, 699-707.	2.0	4
70	Sol-Gel Ru/SiO2-Catalysts: Theoretical and Experimental Determination of the Ru-in-Silica Structures. Journal of Catalysis, 1993, 141, 114-123.	6.2	23
71	Theoretical study of the interaction of Ga. Ga+, and Ga2+ with the hydrogen molecule. International Journal of Quantum Chemistry, 1992, 44, 781-791.	2.0	5
72	Role of excited states of maximal d-shell occupancy in the Ru + H2 reaction. Chemical Physics Letters, 1992, 189, 378-382.	2.6	8

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73	MCSCF+MRCI study of the interaction of Zn, Zn+ and Zn2+ with the hydrogen molecule. Chemical Physics Letters, 1991, 186, 107-112.	2.6	20