Elizabeth Florez

List of Publications by Year
in descending order

58 papers	1,594 citations	304743 22 h-index	315739 38 g-index
59 all docs	59 docs citations	59 times ranked	1768 citing authors

#	Article	IF	Citations
1	Not a Mere Decoration: Impact of Submonolayer Coverages of Nickel on Fundamental Properties of Platinum. Journal of Physical Chemistry C, 2022, 126, 10167-10180.	3.1	3
2	Not all platinum surfaces are the same: Effect of the support on fundamental properties of platinum adlayer and its implications for the activity toward hydrogen evolution reaction. Electrochimica Acta, 2021, 368, 137598.	5.2	9
3	Utilization of water hyacinth (Eichhornia crassipes) rejects as phosphate-rich fertilizer. Journal of Environmental Chemical Engineering, 2021, 9, 104776.	6.7	15
4	Spot the difference: hydrogen adsorption and dissociation on unsupported platinum and platinum-coated transition metal carbides. Physical Chemistry Chemical Physics, 2021, 23, 20255-20267.	2.8	10
5	Size and Stoichiometry Effects on the Reactivity of MoC_y Nanoparticles toward Ethylene. Journal of Physical Chemistry C, 2021, 125, 6287-6297.	3.1	5
6	Pushing Cu uphill of the volcano curve: Impact of a WC support on the catalytic activity of copper toward the hydrogen evolution reaction. International Journal of Hydrogen Energy, 2021, 46, 25092-25102.	7.1	7
7	Phosphorene and phosphorene oxides as a toxic gas sensor materials: a theoretical study. Journal of Physics Condensed Matter, 2021, 33, 455501.	1.8	6
8	Recovering phosphorus from aqueous solutions using water hyacinth (Eichhornia crassipes) toward sustainability through its transformation to apatite. Journal of Environmental Chemical Engineering, 2021, 9, 106225.	6.7	13
9	Understanding mechanisms in the adsorption of lead and copper ions on chili seed waste in single and multicomponent systems: a combined experimental and computational study. Environmental Science and Pollution Research, 2021, 28, 23204-23219.	5.3	10
10	To be or not to be? that is the entropic, enthalpic, and molecular interaction dilemma in theÂ formation of (water)20 clusters and methane clathrate. ChemPhysChem, 2021, , .	2.1	4
11	CO2 activation on small Cu-Ni and Cu-Pd bimetallic clusters. Molecular Catalysis, 2020, 484, 110733.	2.0	22
12	Toward the design of efficient adsorbents for Hg 2+ removal: Molecular and thermodynamic insights. International Journal of Quantum Chemistry, 2020, 120, e26258.	2.0	5
13	Critical Hydrogen Coverage Effect on the Hydrogenation of Ethylene Catalyzed by Î´-MoC(001): An Ab Initio Thermodynamic and Kinetic Study. ACS Catalysis, 2020, 10, 6213-6222.	11.2	21
14	Promoting effect of tungsten carbide on the catalytic activity of Cu for CO₂ reduction. Physical Chemistry Chemical Physics, 2020, 22, 13666-13679.	2.8	16
15	Removal of Cr (VI) from an aqueous solution using an activated carbon obtained from teakwood sawdust: Kinetics, equilibrium, and density functional theory calculations. Journal of Environmental Chemical Engineering, 2020, 8, 103702.	6.7	51
16	Role of Transition Metals on TM/Mo2C Composites: Hydrogen Evolution Activity in Mildly Acidic and Alkaline Media. ACS Applied Materials & Interfaces, 2020, 12, 27150-27165.	8.0	20
17	Microsolvation of small cations and anions. International Journal of Quantum Chemistry, 2019, 119, e25766.	2.0	26
18	Binding and activation of ethylene on tungsten carbide and platinum surfaces. Physical Chemistry Chemical Physics, 2019, 21, 17332-17342.	2.8	9

#	Article	IF	Citations
19	A Comprehensive Picture of the Structures, Energies, and Bonding in [SO₄(H₂O)_n]^{2â€“}, n = 1â€“6. Journal of Physical Chemistry A, 2019, 123, 8650-8656.	2.5	12
20	CO, CO2, and H2 Interactions with (0001) and (001) Tungsten Carbide Surfaces: Importance of Carbon and Metal Sites. Journal of Physical Chemistry C, 2019, 123, 8871-8883.	3.1	30
21	Microsolvation of F^{â˜}. Physical Chemistry Chemical Physics, 2018, 20, 8909-8916.	2.8	24
22	Adsorption of Nitrate and Bicarbonate on Fe-(Hydr)oxide. Inorganic Chemistry, 2017, 56, 5455-5464.	4.0	22
23	Acetylene adsorption on Î´-MoC(001), TiC(001) and ZrC(001) surfaces: a comprehensive periodic DFT study. Physical Chemistry Chemical Physics, 2017, 19, 1571-1579.	2.8	13
24	Acetylene and Ethylene Adsorption on a Î²-Mo₂C(100) Surface: A Periodic DFT Study on the Role of C- and Mo-Terminations for Bonding and Hydrogenation Reactions. Journal of Physical Chemistry C, 2017, 121, 19786-19795.	3.1	22
25	Structure and bonding in WC n (nÂ=Â2â€“5) clusters. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	1
26	Microsolvation of NO₃^{â˜}: structural exploration and bonding analysis. RSC Advances, 2016, 6, 71913-71923.	3.6	37
27	Systematic Theoretical Study of Ethylene Adsorption on Î´-MoC(001), TiC(001), and ZrC(001) Surfaces. Journal of Physical Chemistry C, 2016, 120, 13531-13540.	3.1	19
28	Unusual solvation through both p-orbital lobes of a carbene carbon. Journal of Chemical Physics, 2015, 142, 094302.	3.0	5
29	Phosphorus recovery through struvite precipitation from wastewater: effect of the competitive ions. Desalination and Water Treatment, 2015, 54, 2468-2479.	1.0	42
30	Potential Energy Surfaces of WC₆ Clusters in Different Spin States. Journal of Physical Chemistry A, 2014, 118, 5762-5768.	2.5	12
31	Density functional theory characterization of phosphate and sulfate adsorption on Fe-(hydr)oxide: Reactivity, pH effect, estimation of Gibbs free energies, and topological analysis of hydrogen bonds. Computational and Theoretical Chemistry, 2013, 1005, 16-24.	2.5	54
32	Theoretical design of stable small aluminiumâ€“magnesium binary clusters. Physical Chemistry Chemical Physics, 2013, 15, 2222-2229.	2.8	26
33	Why is quercetin a better antioxidant than taxifolin? Theoretical study of mechanisms involving activated forms. Journal of Molecular Modeling, 2013, 19, 2165-2172.	1.8	38
34	Microsolvation of Mg2+, Ca2+: strong influence of formal charges in hydrogen bond networks. Journal of Molecular Modeling, 2013, 19, 1763-1777.	1.8	42
35	Topological analysis of tetraphosphorus oxides (P4O6+n (nâ€‰=â€‰0â€“4)). Journal of Molecular Modeling, 2013, 19, 2057-2067.	1.8	6
36	Theoretical study of the structure and reactivity descriptors of CunM (M Ni, Pd, Pt; n = 1â€“4) bimetallic nanoparticles supported on MgO(001). Surface Science, 2012, 606, 1010-1018.	1.9	15

#	Article	IF	Citations
37	An orbital and electron density analysis of weak interactions in ethanol-water, methanol-water, ethanol and methanol small clusters. Journal of Chemical Physics, 2012, 136, 144306.	3.0	19
38	Reactivity of Transition Metals (Pd, Pt, Cu, Ag, Au) toward Molecular Hydrogen Dissociation: Extended Surfaces versus Particles Supported on TiC(001) or Small Is Not Always Better and Large Is Not Always Bad. Journal of Physical Chemistry C, 2011, 115, 11666-11672.	3.1	82
39	Theoretical Study of the Interaction of CO on TiC(001) and Au Nanoparticles Supported on TiC(001): Probing the Nature of the Au/TiC Interface. Journal of Physical Chemistry C, 2011, 115, 22495-22504.	3.1	17
40	On the dissociation of molecular hydrogen by Au supported on transition metal carbides: choice of the most active support. Physical Chemistry Chemical Physics, 2011, 13, 6865.	2.8	31
41	Novel Auâ€“TiC catalysts for CO oxidation and desulfurization processes. Catalysis Today, 2011, 166, 2-9.	4.4	37
42	Topological Analysis of the Fukui Function. Journal of Chemical Theory and Computation, 2010, 6, 1470-1478.	5.3	103
43	Hydrogenation Reactions on Au/TiC(001): Effects of Auï£¿C Interactions on the Dissociation of H₂. ChemCatChem, 2010, 2, 1219-1222.	3.7	39
44	Theoretical Analysis of the Adsorption of Late Transition-Metal Atoms on the (001) Surface of Early Transition-Metal Carbides. Journal of Physical Chemistry C, 2010, 114, 1622-1626.	3.1	25
45	Estimation of the interaction energy between small molecules and a silica model as an approach for predicting the interaction order between elastomers and silica. Polymer International, 2009, 58, 811-816.	3.1	13
46	A theoretical study of alkali metal atomic clusters: From Li_n to Cs_n (n = 2â€“8). International Journal of Quantum Chemistry, 2009, 109, 1080-1093.	2.0	21
47	Effect of the Support on the Electronic Structure of Au Nanoparticles Supported on Transition Metal Carbides: Choice of the Best Substrate for Au Activation. Journal of Physical Chemistry C, 2009, 113, 19994-20001.	3.1	28
48	Adsorption and diffusion of Au atoms on the (001) surface of Ti, Zr, Hf, V, Nb, Ta, and Mo carbides. Journal of Chemical Physics, 2009, 130, 244706.	3.0	17
49	Chemical reactivity of oxygen vacancies on the MgO surface: Reactions with CO2, NO2 and metals. Catalysis Today, 2008, 133-135, 216-222.	4.4	56
50	Dry reforming of methane over LaNi1â^'yByO3Â±Î´ (B=Mg, Co) perovskites used as catalyst precursor. Applied Catalysis A: General, 2008, 334, 251-258.	4.3	204
51	Stochastic Search of the Quantum Conformational Space of Small Lithium and Bimetallic Lithiumâ^'Sodium Clusters. Journal of Physical Chemistry A, 2008, 112, 5749-5755.	2.5	71
52	Effect of surface site on the spin state of first-row transition metals adsorbed on MgO: Embedded cluster model and hybrid density functional theory calculations. Physical Review B, 2008, 78, .	3.2	6
53	Density functional theory characterization of the formation of copper clusters on Fs and centers on a MgO surface. Surface Science, 2007, 601, 656-664.	1.9	9
54	Effect of Ni and Pd on the Geometry, Electronic Properties, and Active Sites of Copper Clusters. Journal of Physical Chemistry B, 2006, 110, 13793-13798.	2.6	28

#	Article	IF	Citations
55	Effects of metalâ€“support interactions on the electronic structures of metal atoms adsorbed on the perfect and defective MgO(100) surfaces. Surface Science, 2006, 600, 1703-1713.	1.9	36
56	Transition-metal atom adsorption on anFsdefect site of MgO (100) and the interaction with a hydrogen atom. Physical Review B, 2006, 73, .	3.2	11
57	Theoretical Study of the Interaction of Molecular Oxygen with Copper Clusters. Journal of Physical Chemistry A, 2005, 109, 7815-7821.	2.5	62
58	Effect of nanostructuring on the activation of CO₂ on molybdenum carbide nanoparticles. Physical Chemistry Chemical Physics, 0, , .	2.8	7