## Mariana I Rojas

List of Publications by Year in descending order

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MADIANA L POIAS

#	Article	IF	CITATIONS
1	Density functional theory study of a graphene sheet modified with titanium in contact with different adsorbates. Physical Review B, 2007, 76, .	1.1	90
2	Interferents for hydrogen storage on a graphene sheet decorated with nickel: A DFT study. International Journal of Hydrogen Energy, 2011, 36, 3537-3546.	3.8	62
3	The origin of the catalysis of hydrogen peroxide reduction by functionalized graphene surfaces: A density functional theory study. Electrochimica Acta, 2010, 56, 523-530.	2.6	57
4	ls Hydrogen Storage Possible in Metal-Doped Graphite 2D Systems in Conditions Found on Earth?. Physical Review Letters, 2011, 107, 158701.	2.9	52
5	The oxygen and chlorine evolution reactions at titanium oxide electrodes modified with platinum. Electrochimica Acta, 1998, 43, 1785-1794.	2.6	43
6	Electric and structural properties of polymeric graphite carbon nitride (g-C3N4): A Density Functional Theory study. Computational and Theoretical Chemistry, 2016, 1098, 41-49.	1.1	35
7	Simulation Study of Pd Submonolayer Films on Au(hkl) and Pt(hkl) and Their Relationship to Underpotential Deposition. Langmuir, 2000, 16, 9539-9546.	1.6	24
8	First-principles studies of lithium storage in reduced graphite oxide. Electrochimica Acta, 2014, 140, 232-237.	2.6	20
9	The origin of high electrocatalytic activity of hydrogen peroxide reduction reaction by a g-C <sub>3</sub> N <sub>4</sub> /HOPG sensor. Nanoscale, 2017, 9, 11170-11179.	2.8	20
10	Energetic and entropic contributions to the underpotential/overpotential deposition shifts on single crystal surfaces from lattice dynamics. Electrochimica Acta, 2006, 51, 3526-3536.	2.6	19
11	Computer simulation of the effective double layer occurring on a catalyst surface under electro-chemical promotion conditions. Journal of Applied Electrochemistry, 2008, 38, 1065-1073.	1.5	17
12	Off lattice Monte Carlo simulation study for different metal adlayers onto (111) substrates. Surface Science, 2004, 569, 76-88.	0.8	16
13	Kinetic Monte Carlo simulation of Pt discontinuous thin film formation adsorbed on Au. Surface Science, 2005, 581, L109-L114.	0.8	16
14	2D-drop model applied to the calculation of step formation energies on a (111) substrate. Surface Science, 2002, 499, L135-L140.	0.8	10
15	First-principles studies concerning optimization of hydrogen storage in nanoporous reduced graphite oxide. International Journal of Hydrogen Energy, 2014, 39, 4396-4403.	3.8	10
16	Curvature effect in the longitudinal unzipping carbon nanotubes. Journal of Solid State Electrochemistry, 2013, 17, 1189-1200.	1.2	9
17	Influence of coadsorbed H in CO dissociation and CHn formation on Fe(100): A DFT study. Applied Surface Science, 2015, 346, 438-442.	3.1	9
18	A jellium/point dipoles model for water adsorption on Ag(110). Surface Science, 1990, 227, L121-1124.	0.8	8

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19	Kinetics and Mechanism of the Hydrogen Peroxide Reduction Reaction on a Graphite Carbon Nitride Sensor. Journal of Physical Chemistry C, 2020, 124, 336-346.	1.5	8
20	Theoretical Study about the Adsorption of Lead on (111), (100), (110) Monocrystalline Surfaces of Gold. Zeitschrift Fur Physikalische Chemie, 1994, 185, 33-50.	1.4	6
21	Monte Carlo Simulation of Properties of Monolayers and Metal Islands Adsorbed on Metallic (111) Surfaces. Langmuir, 2004, 20, 4279-4288.	1.6	6
22	Computer simulation of reversible electrochemical catalyst promoter dosing. Electrochimica Acta, 2010, 55, 8673-8679.	2.6	5
23	An extended Hückel/point dipole model for the calculation of dipole potentials for sp metals. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1991, 303, 55-63.	0.3	4
24	A new model for the prediction of oxygen interference in hydrogen storage systems. International Journal of Hydrogen Energy, 2014, 39, 5899-5905.	3.8	4
25	Differentiated interactions in phosphate solutions: Comparing Ag(111) and Ag(100) surfaces. Journal of Electroanalytical Chemistry, 2017, 799, 487-496.	1.9	4
26	Experimental and vdW-DFT Study of the Structure, Properties, and Stability of Isonicotinic Acid Self-Assembled Monolayers on Gold. Journal of Physical Chemistry C, 2016, 120, 4364-4372.	1.5	3
27	Morphological and electrochemical characterizations of a carbon nitride/highly oriented pyrolytic graphite electrode. Journal of Electroanalytical Chemistry, 2021, 898, 115621.	1.9	3
28	A theoretical study on the stability of different submonolayers or a monolayer of lead adsorbed on Au(100). Journal of Electroanalytical Chemistry, 1996, 405, 33-38.	1.9	2
29	Off lattice Monte-Carlo simulations of low-dimensional surface defects and metal deposits on Pt(111). Electrochemistry Communications, 2005, 7, 472-476.	2.3	2
30	Changes in electronic structure of graphene by adsorption of low melamine coverages. Surface Science, 2022, 723, 122120.	0.8	2
31	Specific adsorption of phosphate species on Ag (111) and Ag (100) electrodes and their effect at low overpotentials of the hydrogen evolution reaction. Applied Surface Science Advances, 2021, 3, 100041.	2.9	0