Ezequiel Pedro Marcos Leiva

List of Publications by Citations

140 papers	2,236 citations	24 h-index	36 g-index
145 ext. papers	2,416 ext. citations	4.3 avg, IF	5.03 L-index

#	Paper	IF	Citations
140	Density functional theory study of a graphene sheet modified with titanium in contact with different adsorbates. *Physical Review B*, **2007**, 76,	3.3	85
139	Collision as a way of forming bimetallic nanoclusters of various structures and chemical compositions. *Journal of Chemical Physics*, **2005**, 123, 184505	3.9	81
138	Potentiodynamic and AC Impedance Investigation of Anodic Zirconium Oxide Films. *Journal of the Electrochemical Society*, **1990**, 137, 524-530	3.9	59
137	Interferents for hydrogen storage on a graphene sheet decorated with nickel: A DFT study. *International Journal of Hydrogen Energy*, **2011**, 36, 3537-3546	6.7	53
136	CO adsorbate on Pt(111) single crystal surfaces. *Electrochimica Acta*, **1991**, 36, 555-561	6.7	52
135	The origin of the catalysis of hydrogen peroxide reduction by functionalized graphene surfaces: A density functional theory study. *Electrochimica Acta*, **2010**, 56, 523-530	6.7	50
134	Is hydrogen storage possible in metal-doped graphite 2D systems in conditions found on Earth?. *Physical Review Letters*, **2011**, 107, 158701	7.4	49
133	The effect of adsorbed carbon monoxide on hydrogen adsorption and hydrogen evolution on platinum. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1986**, 215, 357-367		48
132	Effect of chain stiffness on the morphology of polyelectrolyte complexes. A Monte Carlo simulation study. *Polymer*, **2010**, 51, 3293-3302	3.9	39
131	Lithium titanate as anode material for lithium ion batteries: Synthesis, post-treatment and its electrochemical response. *Journal of Electroanalytical Chemistry*, **2017**, 799, 142-155	4.1	38
130	Assessment of the potential for hydrogen production from renewable resources in Argentina. *International Journal of Hydrogen Energy*, **2014**, 39, 8204-8214	6.7	37
129	An embedded atom approach to underpotential deposition phenomena. *Surface Science*, **1999**, 421, 59-72	2.8	37
128	Quantitative study of non-covalent interactions at the electrode-electrolyte interface using cyanide-modified Pt(111) electrodes. *ChemPhysChem*, **2011**, 12, 2230-4	3.2	36
127	The oxygen and chlorine evolution reactions at titanium oxide electrodes modified with platinum. *Electrochimica Acta*, **1998**, 43, 1785-1794	6.7	36
126	Analysis of the potential for hydrogen production in the province of Cdoba, Argentina, from wind resources. *International Journal of Hydrogen Energy*, **2010**, 35, 5952-5956	6.7	35
125	Monte Carlo simulation for the formation and growth of low dimensionality phases during underpotential deposition of Ag on Au(100). *Electrochimica Acta*, **1999**, 45, 699-712	6.7	34
124	Comparative study of CO absorbates for different structures of platinum surfaces. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1987**, 227, 199-211		34

123	Underpotential deposition: From planar surfaces to nanoparticles. *Surface Science*, **2015**, 631, 23-34	1.8	33
122	Cu underpotential deposition on Au(111) and Au(100). Can this be explained in terms of the energetics of the Cu/Au system?. *Electrochimica Acta*, **1999**, 45, 691-697	6.7	30
121	Thermodynamic considerations and computer simulations on the formation of core-shell nanoparticles under electrochemical conditions. *Physical Chemistry Chemical Physics*, **2008**, 10, 3561-8	3.6	28
120	The kinetic origin of the Daumas-H□old model for the Li-ion/graphite intercalation system. *Electrochemistry Communications*, **2018**, 93, 133-137	5.1	27
119	On the generation of metal clusters with the electrochemical scanning tunneling microscope. *Surface Science*, **2005**, 597, 133-155	1.8	26
118	Theoretical Considerations of Electrochemical Phase Formation for an Ideal Frank-van der Merwe System. *Journal of the Electrochemical Society*, **2002**, 149, E109	3.9	26
117	The Influence of Platinum Electrode Surface on the Electroadsorption and Electro-Oxidation of Methanol in Acid Solutions. *Journal of the Electrochemical Society*, **1983**, 130, 1305-1312	3.9	25
116	Wind and solar hydrogen for the potential production of ammonia in the state of Cear□Brazil. *International Journal of Hydrogen Energy*, **2015**, 40, 9917-9923	6.7	24
115	When do nanowires break? A model for the theoretical study of the long-term stability of monoatomic nanowires. *Chemical Physics Letters*, **2008**, 460, 261-265	2.5	24
114	Aggregation of casein micelles by interactions with chitosans: a study by Monte Carlo simulations. *Journal of Agricultural and Food Chemistry*, **2005**, 53, 459-63	5.7	24
113	Energetics of silica lithiation and its applications to lithium ion batteries. *Electrochimica Acta*, **2018**, 259, 1053-1058	6.7	24
112	Underpotential deposition on free nanoparticles: Its meaning and measurement. *Electrochemistry Communications*, **2012**, 16, 1-5	5.1	23
111	Comparative Monte Carlo Study of Monolayer Growth in a Heteroepitaxial System in the Presence of Surface Defects. *Langmuir*, **2003**, 19, 10538-10549	4	23
110	Kinetic Monte Carlo Study of Electrochemical Growth in a Heteroepitaxial System. *Langmuir*, **2002**, 18, 9087-9094	4	23
109	Relevance of Heterometallic Binding Energy for Metal Underpotential Deposition. *Langmuir*, **2001**, 17, 2219-2227	4	23
108	A silica/carbon composite as anode for lithium-ion batteries with a large rate capability: Experiment and theoretical considerations. *Electrochimica Acta*, **2018**, 279, 289-300	6.7	22
107	Theoretical studies of preparation of core□shell nanoparticles by electrochemical metal deposition. *Electrochimica Acta*, **2010**, 55, 8244-8251	6.7	22
106	Polyelectrolyte Adsorption on a Charged Surface. A Study by Monte Carlo Simulations. *Macromolecules*, **2007**, 40, 7336-7342	5.5	22

105	Simulation Study of Pd Submonolayer Films on Au(hkl) and Pt(hkl) and Their Relationship to Underpotential Deposition. *Langmuir*, **2000**, 16, 9539-9546	4	22
104	The basis for the formation of stable metal clusters on an electrode surface. *Nanotechnology*, **2003**, 14, 1009-1013	3.4	21
103	A combined experimental and theoretical study of the generation of palladium clusters on Au(111) with a scanning tunnelling microscope. *Electrochimica Acta*, **2003**, 48, 1287-1294	6.7	20
102	Contribution of the metal to the capacitance of the double layer: a self-consistent calculation including pseudopotentials. *Chemical Physics Letters*, **1991**, 187, 143-148	2.5	20
101	Electrodesorption spectra of residues formed on electrochemically modified polycrystalline platinum from carbon dioxide, formic acid, methanol and ethylene glycol adsorption. *Electrochimica Acta*, **1985**, 30, 1111-1114	6.7	20
100	First principles calculations of mechanical properties of 4,4'-bipyridine attached to Au nanowires. *Physical Review Letters*, **2005**, 95, 045503	7.4	19
99	Role of metal contacts in the mechanical properties of molecular nanojunctions: Comparative ab initio study of Au/1,8-octanedithiol and Au/4,4-bipyridine. *Physical Review B*, **2010**, 81,	3.3	18
98	Energetic and entropic contributions to the underpotential/overpotential deposition shifts on single crystal surfaces from lattice dynamics. *Electrochimica Acta*, **2006**, 51, 3526-3536	6.7	18
97	Changes in surface stress caused by the adsorption of an epitaxial metal monolayer. *Chemical Physics Letters*, **2000**, 320, 393-397	2.5	18
96	First-principles studies of lithium storage in reduced graphite oxide. *Electrochimica Acta*, **2014**, 140, 232-237	6.7	17
95	Shedding Light on the Entropy Change Found for the Transition Stage II-Stage I of Li-Ion Storage in Graphite. *Journal of the Electrochemical Society*, **2017**, 164, A6154-A6157	3.9	17
94	The limits of underpotential deposition in the nanoscale. *Electrochemistry Communications*, **2012**, 21, 14-17	5.1	17
93	Polyelectrolyte Adsorption on a Charged Surface. Free Energy Calculation from Monte Carlo Simulations Using Jarzynski Equality. *Macromolecules*, **2008**, 41, 8267-8274	5.5	17
92	On the occurrence of stable and supersaturated metastable states in metallic core-shell nanoparticles. *Physical Chemistry Chemical Physics*, **2010**, 12, 4580-9	3.6	16
91	Atomistic computer simulations on the generation of bimetallic nanoparticles. *Faraday Discussions*, **2008**, 138, 89-104; discussion 119-35, 433-4	3.6	16
90	Theory of electrochemical monoatomic nanowires. *Physical Review B*, **2006**, 74,	3.3	16
89	Statistical mechanical modeling of the transition Stage II -Stage I of Li-ion storage in graphite. A priori vs induced heterogeneity. *Electrochimica Acta*, **2017**, 245, 569-574	6.7	15
88	A Reversible Molecular Switch Based on the Biphenyl Structure. *Journal of Physical Chemistry C*, **2013**, 117, 25724-25732	3.8	15

87	Configurational Behavior and Conductance of Alkanedithiol Molecular Wires from Accelerated Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2012**, 8, 4539-45	6.4	15
86	On the selective decoration of facets in metallic nanoparticles. *Journal of Materials Research*, **2012**, 27, 1777-1786	2.5	15
85	On the catalytic activity of palladium clusters generated with the electrochemical scanning tunnelling microscope. *Electrochemistry Communications*, **2003**, 5, 584-586	5.1	15
84	Kinetic Monte Carlo simulation of Pt discontinuous thin film formation adsorbed on Au. *Surface Science*, **2005**, 581, L109-L114	1.8	15
83	Thermodynamic derivation and model calculations of the metal underpotential dependence on electron work function differences. *Journal of Electroanalytical Chemistry*, **1993**, 350, 1-14	4.1	15
82	Comparative Study of Different Alkali (Na, Li) Titanate Substrates as Active Materials for Anodes of Lithium - Ion Batteries. *ECS Transactions*, **2014**, 63, 113-128	1	14
81	In silico and in vitro characterization of phospholipase A isoforms from soybean (Glycine max). *Biochimie*, **2012**, 94, 2608-19	4.6	14
80	Properties of rotating nanoalloys formed by cluster collision: a computer simulation study. *Journal of Chemical Physics*, **2011**, 134, 094701	3.9	14
79	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	2.6	14
78	An experimental and theoretical approach on the effect of presence of oxygen in milled graphite as lithium storage material. *Electrochimica Acta*, **2014**, 140, 160-167	6.7	13
77	Model calculations for copper clusters on Au(111) surfaces. *Journal of Electroanalytical Chemistry*, **2002**, 518, 84-90	4.1	13
76	Voltammetric Electro-Oxidation of Carbon Monoxide Previously Adsorbed on Electrochemically Modified Platinum Electrodes. *Journal of the Electrochemical Society*, **1986**, 133, 1660-1662	3.9	13
75	Kinetic Monte Carlo applied to the electrochemical study of the Li-ion graphite system. *Electrochimica Acta*, **2020**, 331, 135439	6.7	13
74	Study of the natural resource and economic feasibility of the production and delivery of wind hydrogen in the province of C doba, Argentina. *International Journal of Hydrogen Energy*, **2015**, 40, 4413-4425	6.7	12
73	Thermodynamic stability of electrochemically decorated Au Pd core@shell nanoparticles. *Electrochimica Acta*, **2012**, 76, 424-429	6.7	12
72	Criticality of the phase transition on stage two in a lattice-gas model of a graphite anode in a lithium-ion battery. *Physical Chemistry Chemical Physics*, **2017**, 19, 23138-23145	3.6	12
71	Anchoring sites to the STM tip can explain multiple peaks in single molecule conductance histograms. *Physical Chemistry Chemical Physics*, **2013**, 15, 1526-31	3.6	12
70	Externally applied electric fields on immiscible lipid monolayers: repulsion between condensed domains precludes domain migration. *Langmuir*, **2006**, 22, 9664-70	4	12

69	Monte Carlo simulation of metal deposition on foreign substrates. *Surface Science*, **2006**, 600, 4741-4751	1.8	12
68	Effect of Temperature on The Kinetics of Electrochemical Insertion of Li-Ions into a Graphite Electrode Studied by Kinetic Monte Carlo. *Journal of the Electrochemical Society*, **2020**, 167, 013533	3.9	12
67	Kinetic Monte Carlo simulations applied to Li-ion and post Li-ion batteries: a key link in the multi-scale chain. *Progress in Energy*, **2021**, 3, 042001	7.7	12
66	Super-Nernstian Shifts of Interfacial Proton-Coupled Electron Transfers: Origin and Effect of Noncovalent Interactions. *Journal of Physical Chemistry C*, **2016**, 120, 15586-15592	3.8	11
65	Grand Canonical Monte Carlo Study of Li Intercalation into Graphite. *Journal of the Electrochemical Society*, **2018**, 165, A2019-A2025	3.9	11
64	On the Stability of Ag/Au(111) Expanded Structures. *Langmuir*, **2002**, 18, 6628-6632	4	11
63	The influence of solution composition on the kinetics of □educed□CO2 electrooxidation at polycrystalline platinum. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1985**, 189, 257-269		11
62	First-principles studies concerning optimization of hydrogen storage in nanoporous reduced graphite oxide. *International Journal of Hydrogen Energy*, **2014**, 39, 4396-4403	6.7	10
61	Electrochemical, HR-XPS and SERS study of the self-assembly of biphenyl 4,4?-dithiol on Au(111) from solution phase. *Surface Science*, **2014**, 630, 101-108	1.8	10
60	A model for underpotential deposition in the presence of anions. *Journal of Chemical Physics*, **2010**, 132, 184703	3.9	10
59	Substituent Effect on the Mechanical Properties of Au□N Nanojunctions. *Journal of Physical Chemistry C*, **2009**, 113, 3850-3854	3.8	10
58	Effects of tip structure on the generation of metal clusters by an STM tip: a way to control the orientation of nanocrystallites?. *Nanotechnology*, **2005**, 16, 974-980	3.4	10
57	Electrochemical behaviour of passive zirconium alloys. *Electrochimica Acta*, **1992**, 37, 281-287	6.7	10
56	Kinetic model for the long term stability of contaminated monoatomic nanowires. *Physical Review B*, **2010**, 81,	3.3	9
55	Stochastic model for spontaneous formation of molecular wires. *Electrochimica Acta*, **2009**, 54, 2977-2982	2.7	9
54	2D-drop model applied to the calculation of step formation energies on a (111) substrate. *Surface Science*, **2002**, 499, L135-L140	1.8	9
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52	Computer simulation of adsorption on nanoparticles: the case of attractive interactions. *Physical Review E*, **2012**, 86, 061602	2.4	8

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50	Spontaneous nanoripple formation on metallic templates. *ACS Nano*, **2008**, 2, 2531-9	16.7	8
49	NEMCA effect: why are the work function changes of the gas exposed catalyst-electrode surface one-to-one related to the changes in the catalyst working electrode potential?. *Journal of Solid State Electrochemistry*, **2003**, 7, 588-592	2.6	8
48	A jellium/point dipoles model for water adsorption on Ag(110). *Surface Science*, **1990**, 227, L121-1124	1.8	8
47	Monomolecular adsorption on nanoparticles with repulsive interactions: a Monte Carlo study. *Physical Chemistry Chemical Physics*, **2016**, 18, 14610-8	3.6	8
46	Time Recovery for a Complex Process Using Accelerated Dynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 1725-34	6.4	7
45	Non-covalent interactions at electrochemical interfaces: one model fits all?. *Physical Chemistry Chemical Physics*, **2014**, 16, 14281-6	3.6	7
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43	Coalescence of Nanoclusters Analyzed by Well-Tempered Metadynamics. Comparison with Straightforward Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 3874-3880	6.4	7
42	Simulated annealing prediction of the crystal structure of ternary inorganic compounds using symmetry restrictions. *Dalton Transactions RSC*, **2000**, 4258-4262		7
41	Semi-empirical calculations of the vibrational frequency of carbon monoxide adsorbed on noble metal single-crystal surfaces. *Journal of Electroanalytical Chemistry*, **1993**, 351, 65-79	4.1	7
40	Complex kinetic behaviour of □educed□CO2 electro-oxidation at Pt electrodes. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1983**, 158, 103-114		7
39	Modeling of lithium-ion batteries is becoming viral: where to go?. *Journal of Solid State Electrochemistry*, **2020**, 24, 2117-2120	2.6	6
38	Mo□e Ha□sinsky: The Discoverer of Underpotential Deposition. *ChemElectroChem*, **2018**, 5, 849-854	4.3	6
37	A Straightforward Approach for the Determination of the Maximum Time Step for the Simulation of Nanometric Metallic Systems. *Journal of Chemical Theory and Computation*, **2012**, 8, 1744-9	6.4	6
36	Low-dimensional metallic nanostructures and their electrochemical relevance: Energetics and phenomenological approach. *Surface Science*, **2006**, 600, 4475-4483	1.8	6
35	Monte Carlo simulation of cluster growth in surface defects induced by the tip of a scanning tunnelling microscope. *Surface Science*, **2004**, 571, L319-L324	1.8	6
34	Inclusion of symmetry for the enhanced determination of crystalline structures from powder diffraction data using simulated annealing. *Chemical Communications*, **1998**, 255-256	5.8	6

33	Theoretical Study about the Adsorption of Lead on (111), (100), (110) Monocrystalline Surfaces of Gold. *Zeitschrift Fur Physikalische Chemie*, **1994**, 185, 33-50	3.1	6
32	Numerical simulations of cyclic voltammetry for lithium-ion intercalation in nanosized systems: finiteness of diffusion versus electrode kinetics. *Journal of Solid State Electrochemistry*, **2020**, 24, 3279-3287	2.6	5
31	Reversible precipitation of casein micelles with a cationic hydroxyethylcellulose. *Journal of Agricultural and Food Chemistry*, **2005**, 53, 9031-8	5.7	5
30	Monte Carlo simulation of properties of monolayers and metal islands adsorbed on metallic (111) surfaces. *Langmuir*, **2004**, 20, 4279-88	4	5
29	Multiple current components for methanol electrosorption and electro-oxidation at platinum in acidic solutions. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1983**, 158, 115-130		5
28	A new model for the prediction of oxygen interference in hydrogen storage systems. *International Journal of Hydrogen Energy*, **2014**, 39, 5899-5905	6.7	4
27	Computer simulation and detailed mean-field approximation applied to adsorption on nanoparticles. *Physical Review E*, **2013**, 88, 062407	2.4	4
26	The behavior of single-molecule junctions predicted by atomistic simulations. *Electrochemistry Communications*, **2009**, 11, 987-989	5.1	4
25	An extended H□kel/point dipole model for the calculation of dipole potentials for sp metals. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1991**, 303, 55-63		4
24	New kinetic insight into the spontaneous oxidation process of lithium in air by EPMA. *Applied Surface Science*, **2016**, 383, 64-70	6.7	4
23	Fractional and integer stages of lithium ion-graphite systems: the role of electrostatic and elastic contributions. *Physical Chemistry Chemical Physics*, **2020**, 22, 16174-16183	3.6	3
22	Underpotential Deposition and Related Phenomena at the Nanoscale: Theory and Applications. *Monographs in Electrochemistry*, **2016**, 277-334	0.8	3
21	Monte Carlo simulation of elongating metallic nanowires in the presence of surfactants. *Journal of Chemical Physics*, **2015**, 143, 244702	3.9	3
20	Mechanical Effects on the Electronic Properties of a Biphenyl-Based Molecular Switch. *Journal of Physical Chemistry C*, **2015**, 119, 5090-5097	3.8	3
19	Diffusion mechanisms taking place at the early stages of cobalt deposition on Au(111). *Journal of Physics Condensed Matter*, **2008**, 20, 265010	1.8	3
18	On the Reasons for Stepwise Changes in the Tunneling Current across Metallic Nanogaps. *Nano Letters*, **2003**, 3, 1633-1637	11.5	3
17	Thermodynamics of Nanoparticle Coalescence at Different Temperatures via Well-Tempered Metadynamics. *Journal of Physical Chemistry C*, **2020**, 124, 24009-24016	3.8	3
16	The Role of Tris(2-carboxyethyl)phosphine Reducing Agent in the Controlled Formation of □Alkanedithiols Monolayers on Au(111) with Monocoordinated and Bicoordinated Configurations. *Langmuir*, **2016**, 32, 9428-36	4	3

15	Simulation of selective thermodynamic deposition in nanoholes. *Physical Chemistry Chemical Physics* , **2017**, 19, 1601-1609	3.6	2
14	On the effect of the carbonaceous substrate in the nucleation of Sn nanoparticles for Li-ion anodes: experiments and first principles calculations. *Journal of Solid State Electrochemistry*, **2018**, 22, 1721-1733	2.6	2
13	A New Approach for the Calculation on the Entropic and Free Energy Contributions to Underpotential Deposition. *ECS Transactions*, **2014**, 58, 3-20	1	2
12	Off lattice Monte-Carlo simulations of low-dimensional surface defects and metal deposits on Pt(1 1 1). *Electrochemistry Communications*, **2005**, 7, 472-476	5.1	2
11	Improving the polysulfide barrier by efficient carbon nanofibers coating on separator/cathode for Li-S batteries. *Journal of Solid State Electrochemistry*, **2020**, 24, 2341-2351	2.6	2
10	Characterization of amorphous LiSi structures from ReaxFF accelerated exploration of local minima. *Physical Chemistry Chemical Physics*, **2021**, 23, 16776-16784	3.6	2
9	Hydrogen Evolution Reaction on Nanostructures Electrodes□ Scenario on Stepped Silver Surfaces. *Electrocatalysis*, **2017**, 8, 587-593	2.7	1
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5	On how interactions influence kinetic limitations in alkali-ion batteries. Application to Li-ion intercalation into graphite through voltammetric experiments. *Journal of Solid State Electrochemistry*, **2021**, 25, 2793	2.6	0
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2	Modeling of Metal Electrodeposition at the Nanoscale **2015**, 1-34		
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