

Ezequiel Pedro Marcos Leiva

List of Publications by Year in descending order

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144
papers

2,638
citations

218381

26
h-index

288905

40
g-index

145
all docs

145
docs citations

145
times ranked

2455
citing authors

#	ARTICLE	IF	CITATIONS
1	Density functional theory study of a graphene sheet modified with titanium in contact with different adsorbates. <i>Physical Review B</i> , 2007, 76, .	1.1	90
2	Collision as a way of forming bimetallic nanoclusters of various structures and chemical compositions. <i>Journal of Chemical Physics</i> , 2005, 123, 184505.	1.2	87
3	Potentiodynamic and AC Impedance Investigation of Anodic Zirconium Oxide Films. <i>Journal of the Electrochemical Society</i> , 1990, 137, 524-530.	1.3	71
4	Interferents for hydrogen storage on a graphene sheet decorated with nickel: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2011, 36, 3537-3546.	3.8	62
5	Assessment of the potential for hydrogen production from renewable resources in Argentina. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 8204-8214.	3.8	61
6	Lithium titanate as anode material for lithium ion batteries: Synthesis, post-treatment and its electrochemical response. <i>Journal of Electroanalytical Chemistry</i> , 2017, 799, 142-155.	1.9	60
7	CO adsorbate on Pt(111) single crystal surfaces. <i>Electrochimica Acta</i> , 1991, 36, 555-561.	2.6	59
8	The origin of the catalysis of hydrogen peroxide reduction by functionalized graphene surfaces: A density functional theory study. <i>Electrochimica Acta</i> , 2010, 56, 523-530.	2.6	57
9	Is Hydrogen Storage Possible in Metal-Doped Graphite 2D Systems in Conditions Found on Earth?. <i>Physical Review Letters</i> , 2011, 107, 158701.	2.9	52
10	Analysis of the potential for hydrogen production in the province of Córdoba, Argentina, from wind resources. <i>International Journal of Hydrogen Energy</i> , 2010, 35, 5952-5956.	3.8	51
11	The effect of adsorbed carbon monoxide on hydrogen adsorption and hydrogen evolution on platinum. <i>Journal of Electroanalytical Chemistry and Interfacial Electrochemistry</i> , 1986, 215, 357-367.	0.3	49
12	The oxygen and chlorine evolution reactions at titanium oxide electrodes modified with platinum. <i>Electrochimica Acta</i> , 1998, 43, 1785-1794.	2.6	43
13	Effect of chain stiffness on the morphology of polyelectrolyte complexes. A Monte Carlo simulation study. <i>Polymer</i> , 2010, 51, 3293-3302.	1.8	43
14	Quantitative Study of Non-Covalent Interactions at the Electrode-Electrolyte Interface Using Cyanide-Modified Pt(111) Electrodes. <i>ChemPhysChem</i> , 2011, 12, 2230-2234.	1.0	40
15	Energetics of silica lithiation and its applications to lithium ion batteries. <i>Electrochimica Acta</i> , 2018, 259, 1053-1058.	2.6	40
16	The kinetic origin of the Daumas-Hård model for the Li-ion/graphite intercalation system. <i>Electrochemistry Communications</i> , 2018, 93, 133-137.	2.3	39
17	An embedded atom approach to underpotential deposition phenomena. <i>Surface Science</i> , 1999, 421, 59-72.	0.8	38
18	Comparative study of CO adsorbates for different structures of platinum surfaces. <i>Journal of Electroanalytical Chemistry and Interfacial Electrochemistry</i> , 1987, 227, 199-211.	0.3	37

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19	Wind and solar hydrogen for the potential production of ammonia in the state of Cear� Brazil. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 9917-9923.	3.8	36
20	Monte Carlo simulation for the formation and growth of low dimensionality phases during underpotential deposition of Ag on Au(100). <i>Electrochimica Acta</i> , 1999, 45, 699-712.	2.6	35
21	Underpotential deposition: From planar surfaces to nanoparticles. <i>Surface Science</i> , 2015, 631, 23-34.	0.8	35
22	A silica/carbon composite as anode for lithium-ion batteries with a large rate capability: Experiment and theoretical considerations. <i>Electrochimica Acta</i> , 2018, 279, 289-300.	2.6	34
23	Cu underpotential deposition on Au(111) and Au(100). Can this be explained in terms of the energetics of the Cu/Au system?. <i>Electrochimica Acta</i> , 1999, 45, 691-697.	2.6	31
24	Theoretical Considerations of Electrochemical Phase Formation for an Ideal Frank-van der Merwe System. <i>Journal of the Electrochemical Society</i> , 2002, 149, E109.	1.3	31
25	On the generation of metal clusters with the electrochemical scanning tunneling microscope. <i>Surface Science</i> , 2005, 597, 133-155.	0.8	28
26	Thermodynamic considerations and computer simulations on the formation of core-shell nanoparticles under electrochemical conditions. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 3561.	1.3	28
27	The Influence of Platinum Electrode Surface on the Electroadsorption and Electro�Oxidation of Methanol in Acid Solutions. <i>Journal of the Electrochemical Society</i> , 1983, 130, 1305-1312.	1.3	26
28	Aggregation of Casein Micelles by Interactions with Chitosans: A Study by Monte Carlo Simulations. <i>Journal of Agricultural and Food Chemistry</i> , 2005, 53, 459-463.	2.4	26
29	Underpotential deposition on free nanoparticles: Its meaning and measurement. <i>Electrochemistry Communications</i> , 2012, 16, 1-5.	2.3	26
30	Kinetic Monte Carlo Study of Electrochemical Growth in a Heteroepitaxial System. <i>Langmuir</i> , 2002, 18, 9087-9094.	1.6	25
31	When do nanowires break? A model for the theoretical study of the long-term stability of monoatomic nanowires. <i>Chemical Physics Letters</i> , 2008, 460, 261-265.	1.2	25
32	Effect of Temperature on The Kinetics of Electrochemical Insertion of Li-Ions into a Graphite Electrode Studied by Kinetic Monte Carlo. <i>Journal of the Electrochemical Society</i> , 2020, 167, 013533.	1.3	25
33	Simulation Study of Pd Submonolayer Films on Au(hkl) and Pt(hkl) and Their Relationship to Underpotential Deposition. <i>Langmuir</i> , 2000, 16, 9539-9546.	1.6	24
34	Relevance of Heterometallic Binding Energy for Metal Underpotential Deposition. <i>Langmuir</i> , 2001, 17, 2219-2227.	1.6	24
35	The basis for the formation of stable metal clusters on an electrode surface. <i>Nanotechnology</i> , 2003, 14, 1009-1013.	1.3	23
36	Comparative Monte Carlo Study of Monolayer Growth in a Heteroepitaxial System in the Presence of Surface Defects. <i>Langmuir</i> , 2003, 19, 10538-10549.	1.6	23

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37	Theoretical studies of preparation of core-shell nanoparticles by electrochemical metal deposition. <i>Electrochimica Acta</i> , 2010, 55, 8244-8251.	2.6	23
38	Kinetic Monte Carlo applied to the electrochemical study of the Li-ion graphite system. <i>Electrochimica Acta</i> , 2020, 331, 135439.	2.6	23
39	Kinetic Monte Carlo simulations applied to Li-ion and post Li-ion batteries: a key link in the multi-scale chain. <i>Progress in Energy</i> , 2021, 3, 042001.	4.6	23
40	First Principles Calculations of Mechanical Properties of 4,4'-Bipyridine Attached to Au Nanowires. <i>Physical Review Letters</i> , 2005, 95, 045503.	2.9	22
41	Polyelectrolyte Adsorption on a Charged Surface. A Study by Monte Carlo Simulations. <i>Macromolecules</i> , 2007, 40, 7336-7342.	2.2	22
42	Changes in surface stress caused by the adsorption of an epitaxial metal monolayer. <i>Chemical Physics Letters</i> , 2000, 320, 393-397.	1.2	21
43	A combined experimental and theoretical study of the generation of palladium clusters on Au(111) with a scanning tunnelling microscope. <i>Electrochimica Acta</i> , 2003, 48, 1287-1294.	2.6	21
44	Electrodesorption spectra of residues formed on electrochemically modified polycrystalline platinum from carbon dioxide, formic acid, methanol and ethylene glycol adsorption. <i>Electrochimica Acta</i> , 1985, 30, 1111-1114.	2.6	20
45	Contribution of the metal to the capacitance of the double layer: a self-consistent calculation including pseudopotentials. <i>Chemical Physics Letters</i> , 1991, 187, 143-148.	1.2	20
46	First-principles studies of lithium storage in reduced graphite oxide. <i>Electrochimica Acta</i> , 2014, 140, 232-237.	2.6	20
47	Energetic and entropic contributions to the underpotential/overpotential deposition shifts on single crystal surfaces from lattice dynamics. <i>Electrochimica Acta</i> , 2006, 51, 3526-3536.	2.6	19
48	Polyelectrolyte Adsorption on a Charged Surface. Free Energy Calculation from Monte Carlo Simulations Using Jarzynski Equality. <i>Macromolecules</i> , 2008, 41, 8267-8274.	2.2	19
49	Role of metal contacts in the mechanical properties of molecular nanojunctions: Comparativeab initiostudy of Au/1,8-octanedithiol and Au/4,4-bipyridine. <i>Physical Review B</i> , 2010, 81, .	1.1	19
50	Properties of rotating nanoalloys formed by cluster collision: A computer simulation study. <i>Journal of Chemical Physics</i> , 2011, 134, 094701.	1.2	19
51	Shedding Light on the Entropy Change Found for the Transition Stage II to Stage I of Li-Ion Storage in Graphite. <i>Journal of the Electrochemical Society</i> , 2017, 164, A6154-A6157.	1.3	19
52	Thermodynamic derivation and model calculations of the metal underpotential dependence on electron work function differences. <i>Journal of Electroanalytical Chemistry</i> , 1993, 350, 1-14.	1.9	18
53	Comparative Study of Different Alkali (Na, Li) Titanate Substrates as Active Materials for Anodes of Lithium - Ion Batteries. <i>ECS Transactions</i> , 2014, 63, 113-128.	0.3	18
54	Computer simulation of the effective double layer occurring on a catalyst surface under electro-chemical promotion conditions. <i>Journal of Applied Electrochemistry</i> , 2008, 38, 1065-1073.	1.5	17

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55	The limits of underpotential deposition in the nanoscale. <i>Electrochemistry Communications</i> , 2012, 21, 14-17.	2.3	17
56	Kinetic Monte Carlo simulation of Pt discontinuous thin film formation adsorbed on Au. <i>Surface Science</i> , 2005, 581, L109-L114.	0.8	16
57	Theory of electrochemical monoatomic nanowires. <i>Physical Review B</i> , 2006, 74, .	1.1	16
58	Atomistic computer simulations on the generation of bimetallic nanoparticles. <i>Faraday Discussions</i> , 2008, 138, 89-104.	1.6	16
59	On the occurrence of stable and supersaturated metastable states in metallic core-shell nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4580.	1.3	16
60	A Reversible Molecular Switch Based on the Biphenyl Structure. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25724-25732.	1.5	16
61	Super-Nernstian Shifts of Interfacial Proton-Coupled Electron Transfers: Origin and Effect of Noncovalent Interactions. <i>Journal of Physical Chemistry C</i> , 2016, 120, 15586-15592.	1.5	16
62	Statistical mechanical modeling of the transition Stage II $\hat{\rightarrow}$ Stage I of Li-ion storage in graphite. A priori vs induced heterogeneity. <i>Electrochimica Acta</i> , 2017, 245, 569-574.	2.6	16
63	Grand Canonical Monte Carlo Study of Li Intercalation into Graphite. <i>Journal of the Electrochemical Society</i> , 2018, 165, A2019-A2025.	1.3	16
64	Numerical simulations of cyclic voltammetry for lithium-ion intercalation in nanosized systems: finiteness of diffusion versus electrode kinetics. <i>Journal of Solid State Electrochemistry</i> , 2020, 24, 3279-3287.	1.2	16
65	On the catalytic activity of palladium clusters generated with the electrochemical scanning tunnelling microscope. <i>Electrochemistry Communications</i> , 2003, 5, 584-586.	2.3	15
66	On the selective decoration of facets in metallic nanoparticles. <i>Journal of Materials Research</i> , 2012, 27, 1777-1786.	1.2	15
67	Configurational Behavior and Conductance of Alkanedithiol Molecular Wires from Accelerated Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4539-4545.	2.3	15
68	In silico and in vitro characterization of phospholipase A2 isoforms from soybean (<i>Glycine max</i>). <i>Biochimie</i> , 2012, 94, 2608-2619.	1.3	15
69	An experimental and theoretical approach on the effect of presence of oxygen in milled graphite as lithium storage material. <i>Electrochimica Acta</i> , 2014, 140, 160-167.	2.6	15
70	Study of the natural resource and economic feasibility of the production and delivery of wind hydrogen in the province of C�rdoba, Argentina. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 4413-4425.	3.8	15
71	Voltammetric Electro�Oxidation of Carbon Monoxide Previously Adsorbed on Electrochemically Modified Platinum Electrodes. <i>Journal of the Electrochemical Society</i> , 1986, 133, 1660-1662.	1.3	14
72	Electrochemical behaviour of passive zirconium alloys. <i>Electrochimica Acta</i> , 1992, 37, 281-287.	2.6	13

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73	Model calculations for copper clusters on Au(111) surfaces. <i>Journal of Electroanalytical Chemistry</i> , 2002, 518, 84-90.	1.9	13
74	Monte Carlo simulation of metal deposition on foreign substrates. <i>Surface Science</i> , 2006, 600, 4741-4751.	0.8	13
75	Anchoring sites to the STM tip can explain multiple peaks in single molecule conductance histograms. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1526-1531.	1.3	13
76	Criticality of the phase transition on stage two in a lattice-gas model of a graphite anode in a lithium-ion battery. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23138-23145.	1.3	13
77	Multiple current components for methanol electrosorption and electro-oxidation at platinum in acidic solutions. <i>Journal of Electroanalytical Chemistry and Interfacial Electrochemistry</i> , 1983, 158, 115-130.	0.3	12
78	Externally Applied Electric Fields on Immiscible Lipid Monolayers: Repulsion between Condensed Domains Precludes Domain Migration. <i>Langmuir</i> , 2006, 22, 9664-9670.	1.6	12
79	Thermodynamic stability of electrochemically decorated Au@Pd core@shell nanoparticles. <i>Electrochimica Acta</i> , 2012, 76, 424-429.	2.6	12
80	The influence of solution composition on the kinetics of reduced-CO ₂ electrooxidation at polycrystalline platinum. <i>Journal of Electroanalytical Chemistry and Interfacial Electrochemistry</i> , 1985, 189, 257-269.	0.3	11
81	On the Stability of Ag/Au(111) Expanded Structures. <i>Langmuir</i> , 2002, 18, 6628-6632.	1.6	11
82	Effects of tip structure on the generation of metal clusters by an STM tip: a way to control the orientation of nanocrystallites?. <i>Nanotechnology</i> , 2005, 16, 974-980.	1.3	11
83	Substituent Effect on the Mechanical Properties of Au-N Nanojunctions. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3850-3854.	1.5	11
84	A model for underpotential deposition in the presence of anions. <i>Journal of Chemical Physics</i> , 2010, 132, .	1.2	11
85	Coalescence of Nanoclusters Analyzed by Well-Tempered Metadynamics. Comparison with Straightforward Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3874-3880.	2.3	11
86	Complex kinetic behaviour of reduced-CO ₂ electro-oxidation at Pt electrodes. <i>Journal of Electroanalytical Chemistry and Interfacial Electrochemistry</i> , 1983, 158, 103-114.	0.3	10
87	2D-drop model applied to the calculation of step formation energies on a (111) substrate. <i>Surface Science</i> , 2002, 499, L135-L140.	0.8	10
88	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?. <i>Journal of Solid State Electrochemistry</i> , 2003, 7, 588-592.	1.2	10
89	Stochastic model for spontaneous formation of molecular wires. <i>Electrochimica Acta</i> , 2009, 54, 2977-2982.	2.6	10
90	First-principles studies concerning optimization of hydrogen storage in nanoporous reduced graphite oxide. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 4396-4403.	3.8	10

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91	Electrochemical, HR-XPS and SERS study of the self-assembly of biphenyl 4,4'-dithiol on Au(111) from solution phase. <i>Surface Science</i> , 2014, 630, 101-108.	0.8	10
92	Kinetic model for the long term stability of contaminated monoatomic nanowires. <i>Physical Review B</i> , 2010, 81, .	1.1	9
93	Curvature effect in the longitudinal unzipping carbon nanotubes. <i>Journal of Solid State Electrochemistry</i> , 2013, 17, 1189-1200.	1.2	9
94	Time Recovery for a Complex Process Using Accelerated Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1725-1734.	2.3	9
95	Counterion condensation on polyelectrolyte chains adsorbed on charged surfaces. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2015, 487, 49-57.	2.3	9
96	Moise Haassinsky: The Discoverer of Underpotential Deposition. <i>ChemElectroChem</i> , 2018, 5, 849-854.	1.7	9
97	A jellium/point dipoles model for water adsorption on Ag(110). <i>Surface Science</i> , 1990, 227, L121-1124.	0.8	8
98	Spontaneous Nanoripple Formation on Metallic Templates. <i>ACS Nano</i> , 2008, 2, 2531-2539.	7.3	8
99	A Straightforward Approach for the Determination of the Maximum Time Step for the Simulation of Nanometric Metallic Systems. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1744-1749.	2.3	8
100	Computer simulation of adsorption on nanoparticles: The case of attractive interactions. <i>Physical Review E</i> , 2012, 86, 061602.	0.8	8
101	Stretching single atom contacts at multiple subatomic step-length. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 12459.	1.3	8
102	Non-covalent interactions at electrochemical interfaces: one model fits all?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14281-14286.	1.3	8
103	Monomolecular adsorption on nanoparticles with repulsive interactions: a Monte Carlo study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14610-14618.	1.3	8
104	Modeling of lithium-ion batteries is becoming viral: where to go?. <i>Journal of Solid State Electrochemistry</i> , 2020, 24, 2117-2120.	1.2	8
105	Semi-empirical calculations of the vibrational frequency of carbon monoxide adsorbed on noble metal single-crystal surfaces. <i>Journal of Electroanalytical Chemistry</i> , 1993, 351, 65-79.	1.9	7
106	Inclusion of symmetry for the enhanced determination of crystalline structures from powder diffraction data using simulated annealing. <i>Chemical Communications</i> , 1998, , 255-256.	2.2	7
107	Simulated annealing prediction of the crystal structure of ternary inorganic compounds using symmetry restrictions. <i>Dalton Transactions RSC</i> , 2000, , 4258-4262.	2.3	7
108	Low-dimensional metallic nanostructures and their electrochemical relevance: Energetics and phenomenological approach. <i>Surface Science</i> , 2006, 600, 4475-4483.	0.8	7

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109	Improving the polysulfide barrier by efficient carbon nanofibers coating on separator/cathode for Li-S batteries. <i>Journal of Solid State Electrochemistry</i> , 2020, 24, 2341-2351.	1.2	7
110	Sodiation Of Hard Carbon: How Separating Enthalpy And Entropy Contributions Can Find Transitions Hidden In The Voltage Profile. <i>ChemPhysChem</i> , 2022, 23, .	1.0	7
111	Theoretical Study about the Adsorption of Lead on (111), (100), (110) Monocrystalline Surfaces of Gold. <i>Zeitschrift Fur Physikalische Chemie</i> , 1994, 185, 33-50.	1.4	6
112	Monte Carlo simulation of cluster growth in surface defects induced by the tip of a scanning tunnelling microscope. <i>Surface Science</i> , 2004, 571, L319-L324.	0.8	6
113	Monte Carlo Simulation of Properties of Monolayers and Metal Islands Adsorbed on Metallic (111) Surfaces. <i>Langmuir</i> , 2004, 20, 4279-4288.	1.6	6
114	Reversible Precipitation of Casein Micelles with a Cationic Hydroxyethylcellulose. <i>Journal of Agricultural and Food Chemistry</i> , 2005, 53, 9031-9038.	2.4	6
115	Thermodynamics of Nanoparticle Coalescence at Different Temperatures via Well-Tempered Metadynamics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24009-24016.	1.5	6
116	Role of the solvent in the activation of Li_2S as cathode material: a DFT study. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 344003.	0.7	6
117	On how interactions influence kinetic limitations in alkali-ion batteries. Application to Li-ion intercalation into graphite through voltammetric experiments. <i>Journal of Solid State Electrochemistry</i> , 2021, 25, 2793-2806.	1.2	6
118	Voltammetric Behaviour of LMO at the Nanoscale: A Map of Reversibility and Diffusional Limitations. <i>ChemPhysChem</i> , 2022, 23, .	1.0	6
119	Fast charging of alkali-ion batteries at the single-particle level: the impact of particle geometry on diffusional and kinetic bottlenecks in voltammetry. <i>Journal of Solid State Electrochemistry</i> , 2022, 26, 1995-2003.	1.2	6
120	The behavior of single-molecule junctions predicted by atomistic simulations. <i>Electrochemistry Communications</i> , 2009, 11, 987-989.	2.3	5
121	Mechanical Effects on the Electronic Properties of a Biphenyl-Based Molecular Switch. <i>Journal of Physical Chemistry C</i> , 2015, 119, 5090-5097.	1.5	5
122	Fractional and integer stages of lithium ion-graphite systems: the role of electrostatic and elastic contributions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16174-16183.	1.3	5
123	An extended Hückel/point dipole model for the calculation of dipole potentials for sp metals. <i>Journal of Electroanalytical Chemistry and Interfacial Electrochemistry</i> , 1991, 303, 55-63.	0.3	4
124	Computer simulation and detailed mean-field approximation applied to adsorption on nanoparticles. <i>Physical Review E</i> , 2013, 88, 062407.	0.8	4
125	A new model for the prediction of oxygen interference in hydrogen storage systems. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 5899-5905.	3.8	4
126	A New Approach for the Calculation on the Entropic and Free Energy Contributions to Underpotential Deposition. <i>ECS Transactions</i> , 2014, 58, 3-20.	0.3	4

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127	New kinetic insight into the spontaneous oxidation process of lithium in air by EPMA. Applied Surface Science, 2016, 383, 64-70.	3.1	4
128	Underpotential Deposition and Related Phenomena at the Nanoscale: Theory and Applications. Monographs in Electrochemistry, 2016, , 277-334.	0.2	4
129	Hydrogen Evolution Reaction on Nanostructures Electrodesâ€”a Scenario on Stepped Silver Surfaces. Electrocatalysis, 2017, 8, 587-593.	1.5	4
130	Characterization of amorphous Li _x Si structures from ReaxFF <i>via</i> accelerated exploration of local minima. Physical Chemistry Chemical Physics, 2021, 23, 16776-16784.	1.3	4
131	On the Reasons for Stepwise Changes in the Tunneling Current across Metallic Nanogaps. Nano Letters, 2003, 3, 1633-1637.	4.5	3
132	Diffusion mechanisms taking place at the early stages of cobalt deposition on Au(111). Journal of Physics Condensed Matter, 2008, 20, 265010.	0.7	3
133	Monte Carlo simulation of elongating metallic nanowires in the presence of surfactants. Journal of Chemical Physics, 2015, 143, 244702.	1.2	3
134	The Role of Tris(2-carboxyethyl)phosphine Reducing Agent in the Controlled Formation of $\sqrt{3}\times\sqrt{3}$ -Alkanedithiols Monolayers on Au(111) with Monocoordinated and Bicoordinated Configurations. Langmuir, 2016, 32, 9428-9436.	1.6	3
135	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
136	Simulation of selective thermodynamic deposition in nanoholes. Physical Chemistry Chemical Physics, 2017, 19, 1601-1609.	1.3	2
137	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.	1.2	2
138	Computer Simulations of Electrochemical Low-Dimensional Metal Phase Formation. , 0, , 30-60.		1
139	Comment on "Surface thermodynamics reconsidered. Derivation of the Gokhshtein relations from the Gibbs potential; and a new approach to surface stress" by Stephen Fletcher. Journal of Solid State Electrochemistry, 2014, 18, 2837-2839.	1.2	1
140	Computational study of nanostructured materials. Current Opinion in Electrochemistry, 2017, 1, 1-6.	2.5	1
141	Surface Reactivity of Lithium (Poly)sulfides in a Polarizable Environment from First Principles. Topics in Catalysis, 2022, 65, 966-978.	1.3	1
142	What Is Coming Next?. Monographs in Electrochemistry, 2016, , 335-348.	0.2	0
143	Modeling of Metal Electrodeposition at the Nanoscale. , 2015, , 1-34.		0
144	Modeling of Metal Electrodeposition at the Nanoscale. , 2016, , 971-1009.		0