Fabio Negreiros Ribeiro

List of Publications by Year
in descending order

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55 papers	1,700 citations	331538 21 h-index	289141 40 g-index
56 all docs	56 docs citations	56 times ranked	2808 citing authors

#	Article	IF	Citations
1	Interaction of Na with 2D WO₃ and MoO₃ Layers on Pd(100): From Doping to 2D Bronze Formation. Journal of Physical Chemistry C, 2022, 126, 3289-3300.	1.5	5
2	Ab initio atomistic description of temperature-induced phase changes: The cases of zirconia and Ti-Y-co-doped zirconia. Physical Review Materials, 2021, 5, .	0.9	2
3	Predictions of Chemical Shifts for Reactive Intermediates in CO2 Reduction under Operando Conditions. ACS Applied Materials & Interfaces, 2021, 13, 31554-31560.	4.0	12
4	MoS₂ Effect on Nickel Electrochemical Activation: An Atomistic/Experimental Approach. Journal of Physical Chemistry C, 2021, 125, 18640-18652.	1.5	2
5	Iron and oxygen vacancies at the hematite surface: pristine case and with a chlorine adatom. Physical Chemistry Chemical Physics, 2020, 22, 25380-25389.	1.3	7
6	Ultrathin WO₃ Bilayer on Ag(100): A Model for the Structure of 2D WO₃ Nanosheets. Journal of Physical Chemistry C, 2019, 123, 27584-27593.	1.5	11
7	The unexpected effect of vacancies and wrinkling on the electronic properties of MoS₂ layers. Physical Chemistry Chemical Physics, 2019, 21, 24731-24739.	1.3	5
8	Bimetallic Agâ€Pt Subâ€nanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie, 2018, 130, 1223-1227.	1.6	3
9	Bimetallic Agâ€Pt Subâ€nanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie - International Edition, 2018, 57, 1209-1213.	7.2	47
10	Dynamical Solvent Effects on the Charge and Reactivity of Ceria-Supported Pt Nanoclusters. Journal of Physical Chemistry C, 2018, 122, 27507-27515.	1.5	10
11	Interaction of Water with the Gypsum (010) Surface: Structure and Dynamics from Nonlinear Vibrational Spectroscopy and Ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2018, 140, 17141-17152.	6.6	19
12	Ambient-pressure CVD of graphene on low-index Ni surfaces using methane: A combined experimental and first-principles study. Physical Review Materials, 2018, 2, .	0.9	12
13	Alumina-supported sub-nanometer Pt₁₀ clusters: amorphization and role of the support material in a highly active CO oxidation catalyst. Journal of Materials Chemistry A, 2017, 5, 4923-4931.	5.2	72
14	Surface Fe vacancy defects on haematite and their role in light-induced water splitting in artificial photosynthesis. Physical Chemistry Chemical Physics, 2017, 19, 31410-31417.	1.3	12
15	Nanoscale Domain Structure and Defects in a 2-D WO₃ Layer on Pd(100). Journal of Physical Chemistry C, 2016, 120, 28682-28693.	1.5	21
16	Atomistic and Electronic Structure Methods for Nanostructured Oxide Interfaces. Springer Series in Materials Science, 2016, , 39-90.	0.4	4
17	Catalytic Proton Dynamics at the Water/Solid Interface of Ceria-Supported Pt Clusters. Journal of the American Chemical Society, 2016, 138, 11560-11567.	6.6	82
18	Creating single-atom Pt-ceria catalysts by surface step decoration. Nature Communications, 2016, 7, 10801.	5.8	388

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19	Effect of Charges on the Interaction of a Water Molecule with the Fe₂O₃(0001) Surface. Journal of Physical Chemistry C, 2016, 120, 11918-11925.	1.5	22
20	The quantum mechanics derived atomistic mechanism underlying the acceleration of catalytic CO oxidation on Pt(110) by surface acoustic waves. Journal of Materials Chemistry A, 2016, 4, 12036-12045.	5.2	7
21	Reactivity of atomically dispersed Pt²⁺ species towards H₂: model Ptâ€“CeO₂ fuel cell catalyst. Physical Chemistry Chemical Physics, 2016, 18, 7672-7679.	1.3	61
22	The atomistic origin of the extraordinary oxygen reduction activity of Pt₃Ni₇fuel cell catalysts. Chemical Science, 2015, 6, 3915-3925.	3.7	53
23	Effects of Thermal Fluctuations on the Hydroxylation and Reduction of Ceria Surfaces by Molecular H₂. Journal of Physical Chemistry C, 2015, 119, 21567-21573.	1.5	50
24	Ligand/cluster/support catalytic complexes in heterogeneous ultrananocatalysis: NO oxidation on Ag₃/MgO(100). Physical Chemistry Chemical Physics, 2014, 16, 26570-26577.	1.3	10
25	Concepts in theoretical heterogeneous ultrananocatalysis. Comptes Rendus Chimie, 2014, 17, 625-633.	0.2	26
26	Metal Tungstates at the Ultimate Two-Dimensional Limit: Fabrication of a CuWO₄ Nanophase. ACS Nano, 2014, 8, 3947-3954.	7.3	53
27	Role of Cluster Morphology in the Dynamics and Reactivity of Subnanometer Pt Clusters Supported on Ceria Surfaces. Journal of Physical Chemistry C, 2014, 118, 21014-21020.	1.5	47
28	Redox processes at a nanostructured interface under strong electric fields. Nanoscale, 2014, 6, 10589-10595.	2.8	4
29	Atomistic Quantum Plasmonics of Gold Nanowire Arrays. ACS Photonics, 2014, 1, 315-322.	3.2	13
30	Communication: Striking dependence of diffusion kinetics in Agâ€“Cu nanoalloys upon composition and quantum effects. Journal of Chemical Physics, 2014, 141, 041108.	1.2	10
31	Reactivity and catalysis by nanoalloys. , 2013, , 283-344.		1
32	Atomic structure of the Au(110)c(2 Ã— 2)â€“Sb system: A combined LEED and DFT study. Surface Science, 2013, 609, 100-105.	0.8	2
33	Electronic excited states at ultrathin dielectric-metal interfaces. Physical Review B, 2013, 88, .	1.1	5
34	Communication: Kinetics of chemical ordering in Ag-Au and Ag-Ni nanoalloys. Journal of Chemical Physics, 2013, 139, 111102.	1.2	29
35	Direct atomic imaging and density functional theory study of the Au24Pd1 cluster catalyst. Nanoscale, 2013, 5, 9620.	2.8	37
36	Adsorptionâ€Induced Restructuring and Early Stages of Carbonâ€Nanotube Growth on Ni Nanoparticles. Chemistry - A European Journal, 2013, 19, 406-413.	1.7	2

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37	Nanostripe Pattern of NaCl Layers on Cu(110). Physical Review Letters, 2013, 110, 216101.	2.9	18
38	Modelling the metal-on-top effect for Pd clusters on the MgO{100} substrate. Journal of Chemical Physics, 2013, 138, 224703.	1.2	11
39	Computational Approaches to the Chemical Conversion of Carbon Dioxide. ChemSusChem, 2013, 6, 944-965.	3.6	144
40	Ordered Arrays of Size-Selected Oxide Nanoparticles. Physical Review Letters, 2012, 108, 195507.	2.9	21
41	Experimental Evidence and Modified Growth Model of Alloying in In_xGa_{1â€“x}As Nanowires. Journal of Physical Chemistry C, 2012, 116, 24777-24783.	1.5	14
42	CO Oxidation by Subnanometer Ag_xAu_{3â€“x} Supported Clusters via Density Functional Theory Simulations. ACS Catalysis, 2012, 2, 1860-1864.	5.5	57
43	Kinetics of chemical ordering in a Ag-Pt nanoalloy particle via first-principles simulations. Journal of Chemical Physics, 2012, 137, 194302.	1.2	21
44	Work Function of Oxide Ultrathin Films on the Ag(100) Surface. Journal of Chemical Theory and Computation, 2012, 8, 629-638.	2.3	24
45	A first-principles theoretical approach to heterogeneous nanocatalysis. Nanoscale, 2012, 4, 1208-1219.	2.8	47
46	Structure and Bonding of Tungsten Oxide Clusters on Nanostructured Cu-O Surfaces. Journal of Physical Chemistry C, 2011, 115, 23480-23487.	1.5	30
47	Interface Effects on the Magnetism of CoPt-Supported Nanostructures. Nano Letters, 2011, 11, 5542-5547.	4.5	27
48	Structures of AgPd nanoclusters adsorbed on MgO(100): A computational study. Surface Science, 2011, 605, 483-488.	0.8	24
49	Surface investigation of Au monolayers on Pd(100). Physical Review B, 2011, 83, .	1.1	7
50	Geometry of the Au(1 1 0)-(1 Ã— 2) missing-row clean surface: A New LEED and DFT study. Surface Science, 2010, 604, 568-573.	0.8	14
51	Simulation of vacancy diffusion in a silver nanocluster. Chemical Physics Letters, 2010, 498, 312-316.	1.2	14
52	Theoretical study of the heteroepitaxial growth of Pd on Cu(111), Pd on Ni(111), Ni on Pd(111), and Cu on Pd(111) using a semiempirical method. Physical Review B, 2010, 81, .	1.1	4
53	Structures of gas-phase Agâ€“Pd nanoclusters: A computational study. Journal of Chemical Physics, 2010, 132, 234703.	1.2	44
54	Energetics of free pure metallic nanoclusters with different motifs by equivalent crystal theory. Physical Review B, 2007, 76, .	1.1	19

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55	Atomistic modeling of Au-Ag nanoparticle formation. Physical Review B, 2007, 76, .	1.1	14