Alberto Roldan

List of Publications by Year
in descending order

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106 papers	3,959 citations	117625 34 h-index	138484 58 g-index
114 all docs	114 docs citations	114 times ranked	5139 citing authors

#	Article	IF	Citations
1	Dehydrogenation and dehydration of formic acid over orthorhombic molybdenum carbide. Catalysis Today, 2022, 384-386, 197-208.	4.4	13
2	Ostwald ripening microkinetic simulation of Au clusters on MgO(0 0 1). Applied Surface Science, 2022, 572, 151317.	6.1	2
3	The Effect of Pristine and Hydroxylated Oxide Surfaces on the Guaiacol HDO Process: A DFT Study. ChemPhysChem, 2022, 23, .	2.1	6
4	Selective decomposition of hydrazine over metal free carbonaceous materials. Physical Chemistry Chemical Physics, 2022, 24, 3017-3029.	2.8	3
5	Hydrodeoxygenation of guaiacol over orthorhombic molybdenum carbide: a DFT and microkinetic study. Catalysis Science and Technology, 2022, 12, 843-854.	4.1	12
6	Dynamics at Polarized Carbon Dioxideâ€“Iron Oxyhydroxide Interfaces Unveil the Origin of Multicarbon Product Formation. ACS Catalysis, 2022, 12, 411-430.	11.2	19
7	Mechanisms and Trends of Guaiacol Hydrodeoxygenation on Transition Metal Catalysts. Frontiers in Catalysis, 2022, 2, .	3.9	7
8	p-Block Indium Single-Atom Catalyst with Low-Coordinated Inâ€“N Motif for Enhanced Electrochemical CO₂ Reduction. ACS Catalysis, 2022, 12, 7386-7395.	11.2	53
9	CO₂ reduction to acetic acid on the greigite Fe₃S₄{111} surface. Faraday Discussions, 2021, 229, 35-49.	3.2	12
10	Synthesis of palladium-rhodium bimetallic nanoparticles for formic acid dehydrogenation. Journal of Energy Chemistry, 2021, 52, 301-309.	12.9	31
11	Incorporation of nickel single atoms into carbon paper as self-standing electrocatalyst for CO₂reduction. Journal of Materials Chemistry A, 2021, 9, 1583-1592.	10.3	35
12	Controlling the Selectivity of Supported Ru Nanoparticles During Glycerol Hydrogenolysis: Câ^'O vs Câ^'C Cleavage. ChemCatChem, 2021, 13, 1595-1606.	3.7	1
13	Are Carbon-Based Materials Good Supports for the Catalytic Reforming of Ammonia?. Journal of Physical Chemistry C, 2021, 125, 15950-15958.	3.1	10
14	Enhancing activity, selectivity and stability of palladium catalysts in formic acid decomposition: Effect of support functionalization. Catalysis Today, 2021, 382, 61-70.	4.4	16
15	Disclosing the Role of Gold on Palladium â€“ Gold Alloyed Supported Catalysts in Formic Acid Decomposition. ChemCatChem, 2021, 13, 4210-4222.	3.7	16
16	Lowâ€Valence Zn^{Î´+} (0<Î´<2) Singleâ€Atom Material as Highly Efficient Electrocatalyst for CO₂ Reduction. Angewandte Chemie - International Edition, 2021, 60, 22826-22832.	13.8	115
17	Lowâ€Valence Zn^{Î´+} (0<Î´<2) Singleâ€Atom Material as Highly Efficient Electrocatalyst for CO₂ Reduction. Angewandte Chemie, 2021, 133, 23008-23014.	2.0	12
18	Kinetic and mechanistic analysis of NH₃decomposition on Ru(0001), Ru(111) and Ir(111) surfaces. Nanoscale Advances, 2021, 3, 1624-1632.	4.6	19

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19	Stable and Antisintering Tungsten Carbides with Controllable Active Phase for Selective Cleavage of Aryl Ether Câ€“O Bonds. ACS Applied Materials & Interfaces, 2021, 13, 8274-8284.	8.0	4
20	How to go beyond C₁ products with electrochemical reduction of CO₂. Sustainable Energy and Fuels, 2021, 5, 5893-5914.	4.9	19
21	DFT+U Study of the Electronic, Magnetic and Mechanical Properties of Co, CoO, and Co3O4. South African Journal of Chemistry, 2021, 74, .	0.6	2
22	Role of defects in carbon materials during metal-free formic acid dehydrogenation. Nanoscale, 2020, 12, 22768-22777.	5.6	19
23	Biomass hydrodeoxygenation catalysts innovation from atomistic activity predictors. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20200056.	3.4	8
24	The influence of oxygen vacancy and Ce3+ ion positions on the properties of small gold clusters supported on CeO2â^'x(111). Journal of Materials Chemistry A, 2020, 8, 15695-15705.	10.3	17
25	Role of the Support in Gold-Containing Nanoparticles as Heterogeneous Catalysts. Chemical Reviews, 2020, 120, 3890-3938.	47.7	275
26	Mechanistic study of hydrazine decomposition on Ir(111). Physical Chemistry Chemical Physics, 2020, 22, 3883-3896.	2.8	24
27	DFT-Assisted Spectroscopic Studies on the Coordination of Small Ligands to Palladium: From Isolated Ions to Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 4781-4790.	3.1	4
28	Ammonia from Steelworks. Green Energy and Technology, 2020, , 69-80.	0.6	3
29	Tautomerization of Phenol at the External Lewis Acid Sites of Scandium-, Iron- and Gallium-Substituted Zeolite MFI. Journal of Physical Chemistry C, 2019, 123, 7604-7614.	3.1	7
30	The influence of support materials on the structural and electronic properties of gold nanoparticles â€“ a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 19011-19025.	2.8	39
31	Density functional theory study explaining the underperformance of copper oxides as photovoltaic absorbers. Physical Review B, 2019, 99, .	3.2	40
32	Hydrogen adsorption on transition metal carbides: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 5335-5343.	2.8	42
33	A density functional theory study of the hydrogenation and reduction of the thio-spinel Fe₃S₄{111} surface. Physical Chemistry Chemical Physics, 2019, 21, 2426-2433.	2.8	4
34	Carbon dioxide and water co-adsorption on the low-index surfaces of TiC, VC, ZrC and NbC: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 10750-10760.	2.8	25
35	Benzyl alcohol oxidation with Pd-Zn/TiO2: computational and experimental studies. Science and Technology of Advanced Materials, 2019, 20, 367-378.	6.1	26
36	Structural tuning and catalysis of tungsten carbides for the regioselective cleavage of C O bonds. Journal of Catalysis, 2019, 369, 283-295.	6.2	38

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37	Tuning the electronic band gap of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mathvariant="normal">O</mml:mi></mml:mrow></mml:math> via transition metal doping for improved photovoltaic applications. Physical Review Materials, 2019, 3, .	2.4	15
38	Bulk and surface properties of metal carbides: implications for catalysis. Physical Chemistry Chemical Physics, 2018, 20, 6905-6916.	2.8	82
39	Stability and mobility of supported Nin (nÂ= 1â€“10) clusters on ZrO2(111) and YSZ(111) surfaces: a density functional theory study. Faraday Discussions, 2018, 208, 87-104.	3.2	7
40	Hydrogen Generation from Additive-Free Formic Acid Decomposition Under Mild Conditions by Pd/C: Experimental and DFT Studies. Topics in Catalysis, 2018, 61, 254-266.	2.8	68
41	Frontiers in first principles modelling of electrochemical simulations. Current Opinion in Electrochemistry, 2018, 10, 1-6.	4.8	25
42	Reactivity of CO ₂ on the surfaces of magnetite (Fe ₃ O ₄), greigite (Fe ₃ S ₄) and mackinawite (FeS). Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170065.	3.4	27
43	Hydrogen production from formic acid decomposition in the liquid phase using Pd nanoparticles supported on CNFs with different surface properties. Sustainable Energy and Fuels, 2018, 2, 2705-2716.	4.9	37
44	Chemoselective Lactonization of Renewable Succinic Acid with Heterogeneous Nanoparticle Catalysts. ACS Sustainable Chemistry and Engineering, 2018, 6, 16341-16351.	6.7	10
45	CO₂ and H₂ Adsorption and Reaction at Ni_n/YSZ(111) Interfaces: A Density Functional Theory Study. Journal of Physical Chemistry C, 2018, 122, 19463-19472.	3.1	15
46	Platinum Nanoparticle Inclusion into a Carbonized Polymer of Intrinsic Microporosity: Electrochemical Characteristics of a Catalyst for Electroless Hydrogen Peroxide Production. Nanomaterials, 2018, 8, 542.	4.1	8
47	Investigation of the Catalytic Performance of Pd/CNFs for Hydrogen Evolution from Additive-Free Formic Acid Decomposition. Journal of Carbon Research, 2018, 4, 26.	2.7	13
48	CO₂ interaction with violarite (FeNi₂S₄) surfaces: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2018, 20, 20439-20446.	2.8	15
49	Insight into the Nature of Iron Sulfide Surfaces During the Electrochemical Hydrogen Evolution and CO₂ Reduction Reactions. ACS Applied Materials & Interfaces, 2018, 10, 32078-32085.	8.0	33
50	Structures and Properties of As(OH)₃ Adsorption Complexes on Hydrated Mackinawite (FeS) Surfaces: A DFT-D2 Study. Environmental Science & Technology, 2017, 51, 3461-3470.	10.0	49
51	Selective hydrogenation of CO on Fe₃S₄{111}: a computational study. Faraday Discussions, 2017, 197, 325-336.	3.2	7
52	Novel photocatalysts: general discussion. Faraday Discussions, 2017, 197, 533-546.	3.2	1
53	Designing new catalysts for synthetic fuels: general discussion. Faraday Discussions, 2017, 197, 353-388.	3.2	7
54	Density functional theory study of the zeolite-mediated tautomerization of phenol and catechol. Molecular Catalysis, 2017, 433, 334-345.	2.0	14

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55	A kinetic model of water adsorption, clustering and dissociation on the Fe₃S₄{001} surface. Physical Chemistry Chemical Physics, 2017, 19, 12045-12055.	2.8	16
56	Density Functional Theory Study of Ni Clusters Supported on the ZrO₂(111) Surface. Fuel Cells, 2017, 17, 125-131.	2.4	16
57	Micro-kinetic simulations of the catalytic decomposition of hydrazine on the Cu(111) surface. Faraday Discussions, 2017, 197, 41-57.	3.2	14
58	Product tunable behavior of carbon nanotubes-supported Niâ€“Fe catalysts for guaiacol hydrodeoxygenation. Applied Catalysis A: General, 2017, 529, 20-31.	4.3	153
59	Periodic modeling of zeolite Ti-LTA. Journal of Chemical Physics, 2017, 147, 074701.	3.0	11
60	DFT-D2 simulations of water adsorption and dissociation on the low-index surfaces of mackinawite (FeS). Journal of Chemical Physics, 2016, 144, 174704.	3.0	33
61	A density functional theory study of the adsorption behaviour of CO2 on Cu2O surfaces. Journal of Chemical Physics, 2016, 145, 044709.	3.0	55
62	Catalytic water dissociation by greigite Fe ₃ S ₄ surfaces: density functional theory study. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2016, 472, 20160080.	2.1	17
63	Early Oxidation Processes on the Greigite Fe₃S₄(001) Surface by Water: A Density Functional Theory Study. Journal of Physical Chemistry C, 2016, 120, 8616-8629.	3.1	32
64	Surface and shape modification of mackinawite (FeS) nanocrystals by cysteine adsorption: a first-principles DFT-D2 study. Physical Chemistry Chemical Physics, 2016, 18, 32007-32020.	2.8	35
65	DFT Modeling of the Adsorption of Trimethylphosphine Oxide at the Internal and External Surfaces of Zeolite MFI. Journal of Physical Chemistry C, 2016, 120, 19097-19106.	3.1	24
66	DFT-D2 Study of the Adsorption and Dissociation of Water on Clean and Oxygen-Covered {001} and {011} Surfaces of Mackinawite (FeS). Journal of Physical Chemistry C, 2016, 120, 21441-21450.	3.1	34
67	Adsorption of Methyl Acetoacetate at Ni{111}: Experiment and Theory. Journal of Physical Chemistry C, 2016, 120, 27490-27499.	3.1	17
68	Designing new catalysts: synthesis of new active structures: general discussion. Faraday Discussions, 2016, 188, 131-159.	3.2	4
69	Catalyst design from theory to practice: general discussion. Faraday Discussions, 2016, 188, 279-307.	3.2	2
70	Density functional theory study of the interaction of H2O, CO2 and CO with the ZrO2 (111), Ni/ZrO2 (111), YSZ (111) and Ni/YSZ (111) surfaces. Surface Science, 2016, 653, 153-162.	1.9	17
71	Highlights from Faraday Discussion: Designing New Heterogeneous Catalysts, London, UK, April 2016. Chemical Communications, 2016, 52, 8335-8341.	4.1	1
72	Methanol formation from CO₂catalyzed by Fe₃S₄{111}: formate versus hydrocarboxyl pathways. Faraday Discussions, 2016, 188, 161-180.	3.2	29

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73	A density functional theory study of the structure of pure-silica and aluminium-substituted MFI nanosheets. Journal of Solid State Chemistry, 2016, 237, 192-203.	2.9	28
74	CuO Surfaces and CO₂ Activation: A Dispersion-Corrected DFT+U Study. Journal of Physical Chemistry C, 2016, 120, 2198-2214.	3.1	165
75	Multichannel Detection and Differentiation of Explosives with a Quantum Dot Array. ACS Nano, 2016, 10, 1139-1146.	14.6	120
76	Ni Deposition on Yttria-Stabilized ZrO₂(111) Surfaces: A Density Functional Theory Study. Journal of Physical Chemistry C, 2015, 119, 6581-6591.	3.1	22
77	First-principles study of the inversion thermodynamics and electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Fe</mml:mi><mml:msub><mml:mi>M</mml:mi><mml:mi>		

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91	The Role of Hydrogen Bonding and Proton Transfer in the Formation of Uracil Networks on the Gold (100) Surface: A Density Functional Theory Approach. Journal of Physical Chemistry C, 2013, 117, 3949-3957.	3.1	31
92	A comparative DFT study of the mechanical and electronic properties of greigite Fe3S4 and magnetite Fe3O4. Journal of Chemical Physics, 2013, 138, 204712.	3.0	75
93	Adsorption of methylamine on mackinawite (FES) surfaces: A density functional theory study. Journal of Chemical Physics, 2013, 139, 124708.	3.0	45
94	Stability and Quenching of Plasmon Resonance Absorption in Magnetic Gold Nanoparticles. Journal of Physical Chemistry Letters, 2011, 2, 2996-3001.	4.6	5
95	Origin of the size dependence of Au nanoparticles toward molecular oxygen dissociation. Theoretical Chemistry Accounts, 2011, 128, 675-681.	1.4	32
96	Electronic and magnetic structure of bulk cobalt: The Î±, Î², and Îµ-phases from density functional theory calculations. Journal of Chemical Physics, 2010, 133, 024701.	3.0	83
97	Theoretical Simulation of Temperature Programmed Desorption of Molecular Oxygen on Isolated Au Nanoparticles from Density Functional Calculations and Microkinetics Models. Journal of Physical Chemistry C, 2010, 114, 5101-5106.	3.1	13
98	O₂ Activation by Au₅ Clusters Stabilized on Clean and Electron-Rich MgO Stepped Surfaces. Journal of Physical Chemistry C, 2010, 114, 16973-16978.	3.1	33
99	Theoretical Confirmation of the Enhanced Facility to Increase Oxygen Vacancy Concentration in TiO₂by Iron Doping. Journal of Physical Chemistry C, 2010, 114, 6511-6517.	3.1	78
100	O2 adsorption and dissociation on neutral, positively and negatively charged Aun (n = 5â€“79) clusters. Physical Chemistry Chemical Physics, 2010, 12, 10723.	2.8	50
101	Critical Size for O₂ Dissociation by Au Nanoparticles. ChemPhysChem, 2009, 10, 348-351.	2.1	108
102	Influence of the exchangeâ€“correlation potential on the description of the molecular mechanism of oxygen dissociation by Au nanoparticles. Theoretical Chemistry Accounts, 2009, 123, 119-126.	1.4	47
103	On the effectiveness of partial oxidation of propylene by gold: A density functional theory study. Journal of Molecular Catalysis A, 2009, 306, 6-10.	4.8	31
104	Growth and properties of Au nanowires. Molecular Simulation, 2009, 35, 1051-1056.	2.0	4
105	Density functional studies of coinage metal nanoparticles: scalability of their properties to bulk. Theoretical Chemistry Accounts, 2008, 120, 565-573.	1.4	61
106	The chemistry of chlorine on Ag(1 1 1) over the sub-monolayer range: A density functional theory investigation. Surface Science, 2008, 602, 2639-2642.	1.9	9