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	Role of the Support in Gold-Containing Nanoparticles as Heterogeneous Catalysts. Chemical Reviews, 2020, 120, 3890-3938.	47.7	275
2	Bio-inspired CO₂conversion by iron sulfide catalysts under sustainable conditions. Chemical Communications, 2015, 51, 7501-7504.	4.1	188
3	A DFT study of the structures, stabilities and redox behaviour of the major surfaces of magnetite Fe₃O₄. Physical Chemistry Chemical Physics, 2014, 16, 21082-21097.	2.8	178
4	CuO Surfaces and CO₂ Activation: A Dispersion-Corrected DFT+U Study. Journal of Physical Chemistry C, 2016, 120, 2198-2214.	3.1	165
5	Product tunable behavior of carbon nanotubes-supported Niâ€“Fe catalysts for guaiacol hydrodeoxygenation. Applied Catalysis A: General, 2017, 529, 20-31.	4.3	153
6	Multichannel Detection and Differentiation of Explosives with a Quantum Dot Array. ACS Nano, 2016, 10, 1139-1146.	14.6	120
7	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
8	Critical Size for O₂ Dissociation by Au Nanoparticles. ChemPhysChem, 2009, 10, 348-351.	2.1	108
9	A Density Functional Theory Study of the Adsorption of Benzene on Hematite (Î±-Fe2O3) Surfaces. Minerals (Basel, Switzerland), 2014, 4, 89-115.	2.0	105
10	Active Nature of Primary Amines during Thermal Decomposition of Nickel Dithiocarbamates to Nickel Sulfide Nanoparticles. Chemistry of Materials, 2014, 26, 6281-6292.	6.7	86
11	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
12	Bulk and surface properties of metal carbides: implications for catalysis. Physical Chemistry Chemical Physics, 2018, 20, 6905-6916.	2.8	82
13	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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19	Density Functional Theory Study of the Adsorption of Hydrazine on the Perfect and Defective Copper (100), (110), and (111) Surfaces. Journal of Physical Chemistry C, 2014, 118, 26103-26114.	3.1	58
20	A density functional theory study of the adsorption behaviour of CO2 on Cu2O surfaces. Journal of Chemical Physics, 2016, 145, 044709.	3.0	55
21	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
22	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
23	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
24	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
25	Activation and dissociation of CO2 on the (001), (011), and (111) surfaces of mackinawite (FeS): A dispersion-corrected DFT study. Journal of Chemical Physics, 2015, 143, 094703.	3.0	46
26	Adsorption of methylamine on mackinawite (FES) surfaces: A density functional theory study. Journal of Chemical Physics, 2013, 139, 124708.	3.0	45
27	Hydrogen adsorption on transition metal carbides: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 5335-5343.	2.8	42
28	Catalytic Dissociation of Water on the (001), (011), and (111) Surfaces of Violarite, FeNi₂S₄: A DFT-D2 Study. Journal of Physical Chemistry C, 2014, 118, 1958-1967.	3.1	41
29	The surface chemistry of NO_x on mackinawite (FeS) surfaces: a DFT-D2 study. Physical Chemistry Chemical Physics, 2014, 16, 15444-15456.	2.8	40
30	Density functional theory study explaining the underperformance of copper oxides as photovoltaic absorbers. Physical Review B, 2019, 99, .	3.2	40
31	Density functional theory calculations of the hydrazine decomposition mechanism on the planar and stepped Cu(111) surfaces. Physical Chemistry Chemical Physics, 2015, 17, 21533-21546.	2.8	39
32	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
33	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
34	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
35	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
36	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

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37	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
38	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
39	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
40	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
41	Origin of the size dependence of Au nanoparticles toward molecular oxygen dissociation. Theoretical Chemistry Accounts, 2011, 128, 675-681.	1.4	32
42	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
43	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
44	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
45	Synthesis of palladium-rhodium bimetallic nanoparticles for formic acid dehydrogenation. Journal of Energy Chemistry, 2021, 52, 301-309.	12.9	31
46	Methanol formation from CO₂catalyzed by Fe₃S₄{111}: formate versus hydrocarboxyl pathways. Faraday Discussions, 2016, 188, 161-180.	3.2	29
47	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
48	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
49	Gadolinium-Vacancy Clusters in the (111) Surface of Gadolinium-Doped Ceria: A Density Functional Theory Study. Chemistry of Materials, 2015, 27, 7910-7917.	6.7	26
50	Benzyl alcohol oxidation with Pd-Zn/TiO2: computational and experimental studies. Science and Technology of Advanced Materials, 2019, 20, 367-378.	6.1	26
51	Frontiers in first principles modelling of electrochemical simulations. Current Opinion in Electrochemistry, 2018, 10, 1-6.	4.8	25
52	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
53	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
54	Mechanistic study of hydrazine decomposition on Ir(111). Physical Chemistry Chemical Physics, 2020, 22, 3883-3896.	2.8	24

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55	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
56	Hydrazine network on Cu(111) surface: A Density Functional Theory approach. Surface Science, 2015, 637-638, 140-148.	1.9	21
57	Role of defects in carbon materials during metal-free formic acid dehydrogenation. Nanoscale, 2020, 12, 22768-22777.	5.6	19
58	Kinetic and mechanistic analysis of NH₃decomposition on Ru(0001), Ru(111) and Ir(111) surfaces. Nanoscale Advances, 2021, 3, 1624-1632.	4.6	19
59	How to go beyond C₁ products with electrochemical reduction of CO₂. Sustainable Energy and Fuels, 2021, 5, 5893-5914.	4.9	19
60	Dynamics at Polarized Carbon Dioxideâ€“Iron Oxyhydroxide Interfaces Unveil the Origin of Multicarbon Product Formation. ACS Catalysis, 2022, 12, 411-430.	11.2	19
61	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
62	Adsorption of Methyl Acetoacetate at Ni{111}: Experiment and Theory. Journal of Physical Chemistry C, 2016, 120, 27490-27499.	3.1	17
63	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
64	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
65	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
66	Density Functional Theory Study of Ni Clusters Supported on the ZrO₂(111) Surface. Fuel Cells, 2017, 17, 125-131.	2.4	16
67	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
68	Disclosing the Role of Gold on Palladium â€“ Gold Alloyed Supported Catalysts in Formic Acid Decomposition. ChemCatChem, 2021, 13, 4210-4222.	3.7	16
69	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
70	CO₂ interaction with violarite (FeNi₂S₄) surfaces: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2018, 20, 20439-20446.	2.8	15
71	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
72	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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73	Micro-kinetic simulations of the catalytic decomposition of hydrazine on the Cu(111) surface. Faraday Discussions, 2017, 197, 41-57.	3.2	14
74	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
75	New Insights into the Structure of the C-Terminated Î²-Mo₂C (001) Surface from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 19224-19231.	3.1	13
76	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
77	Dehydrogenation and dehydration of formic acid over orthorhombic molybdenum carbide. Catalysis Today, 2022, 384-386, 197-208.	4.4	13
78	CO₂ reduction to acetic acid on the greigite Fe₃S₄{111} surface. Faraday Discussions, 2021, 229, 35-49.	3.2	12
79	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
80	Hydrodeoxygenation of guaiacol over orthorhombic molybdenum carbide: a DFT and microkinetic study. Catalysis Science and Technology, 2022, 12, 843-854.	4.1	12
81	Periodic modeling of zeolite Ti-LTA. Journal of Chemical Physics, 2017, 147, 074701.	3.0	11
82	Chemoselective Lactonization of Renewable Succinic Acid with Heterogeneous Nanoparticle Catalysts. ACS Sustainable Chemistry and Engineering, 2018, 6, 16341-16351.	6.7	10
83	Are Carbon-Based Materials Good Supports for the Catalytic Reforming of Ammonia?. Journal of Physical Chemistry C, 2021, 125, 15950-15958.	3.1	10
84	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
85	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
86	Biomass hydrodeoxygenation catalysts innovation from atomistic activity predictors. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20200056.	3.4	8
87	Selective hydrogenation of CO on Fe₃S₄{111}: a computational study. Faraday Discussions, 2017, 197, 325-336.	3.2	7
88	Designing new catalysts for synthetic fuels: general discussion. Faraday Discussions, 2017, 197, 353-388.	3.2	7
89	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
90	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

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91	Mechanisms and Trends of Guaiacol Hydrodeoxygenation on Transition Metal Catalysts. Frontiers in Catalysis, 2022, 2, .	3.9	7
92	The Effect of Pristine and Hydroxylated Oxide Surfaces on the Guaiacol HDO Process: A DFT Study. ChemPhysChem, 2022, 23, .	2.1	6
93	Stability and Quenching of Plasmon Resonance Absorption in Magnetic Gold Nanoparticles. Journal of Physical Chemistry Letters, 2011, 2, 2996-3001.	4.6	5
94	Growth and properties of Au nanowires. Molecular Simulation, 2009, 35, 1051-1056.	2.0	4
95	Designing new catalysts: synthesis of new active structures: general discussion. Faraday Discussions, 2016, 188, 131-159.	3.2	4
96	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
97	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
98	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
99	Ammonia from Steelworks. Green Energy and Technology, 2020, , 69-80.	0.6	3
100	Selective decomposition of hydrazine over metal free carbonaceous materials. Physical Chemistry Chemical Physics, 2022, 24, 3017-3029.	2.8	3
101	Catalyst design from theory to practice: general discussion. Faraday Discussions, 2016, 188, 279-307.	3.2	2
102	Ostwald ripening microkinetic simulation of Au clusters on MgO(0 0 1). Applied Surface Science, 2022, 572, 151317.	6.1	2
103	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
104	Highlights from Faraday Discussion: Designing New Heterogeneous Catalysts, London, UK, April 2016. Chemical Communications, 2016, 52, 8335-8341.	4.1	1
105	Novel photocatalysts: general discussion. Faraday Discussions, 2017, 197, 533-546.	3.2	1
106	Controlling the Selectivity of Supported Ru Nanoparticles During Glycerol Hydrogenolysis: Câ^'O vs Câ^'C Cleavage. ChemCatChem, 2021, 13, 1595-1606.	3.7	1