Ana BelÃ©n MuÃ±oz GarcÃ-a

List of Publications by Year
in descending order

78 papers	3,202 citations	136950 32 h-index	161849 54 g-index
80 all docs	80 docs citations	80 times ranked	3976 citing authors

#	Article	IF	Citations
1	Dye-sensitized solar cells strike back. Chemical Society Reviews, 2021, 50, 12450-12550.	38.1	240
2	Copper Bipyridyl Redox Mediators for Dye-Sensitized Solar Cells with High Photovoltage. Journal of the American Chemical Society, 2016, 138, 15087-15096.	13.7	239
3	Unveiling Structureâ€“Property Relationships in Sr₂Fe_{1.5}Mo_{0.5}O_{6â^Î´}, an Electrode Material for Symmetric Solid Oxide Fuel Cells. Journal of the American Chemical Society, 2012, 134, 6826-6833.	13.7	172
4	Ab Initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in La_{1-x}Sr_xFeO_{3-Î´}(x= 0, 0.25, 0.50). Chemistry of Materials, 2013, 25, 3011-3019.	6.7	153
5	Oxygen Transport in Perovskite-Type Solid Oxide Fuel Cell Materials: Insights from Quantum Mechanics. Accounts of Chemical Research, 2014, 47, 3340-3348.	15.6	121
6	Effect of Antisite Defects on the Formation of Oxygen Vacancies in Sr₂FeMoO₆: Implications for Ion and Electron Transport. Chemistry of Materials, 2011, 23, 4525-4536.	6.7	108
7	Unveiling the controversial mechanism of reversible Na storage in TiO2 nanotube arrays: Amorphous versus anatase TiO2. Nano Research, 2017, 10, 2891-2903.	10.4	90
8	First-Principles Design of New Electrodes for Proton-Conducting Solid-Oxide Electrochemical Cells: A-Site Doped Sr₂Fe_{1.5}Mo_{0.5}O_{6â^Î´} Perovskite. Chemistry of Materials, 2016, 28, 490-500.	6.7	86
9	Combined Structural, Chemometric, and Electrochemical Investigation of Vertically Aligned TiO₂ Nanotubes for Na-ion Batteries. ACS Omega, 2018, 3, 8440-8450.	3.5	86
10	First-Principles Study of Lanthanum Strontium Manganite: Insights into Electronic Structure and Oxygen Vacancy Formation. Journal of Physical Chemistry C, 2014, 118, 13346-13356.	3.1	82
11	Ab initio DFT+U analysis of oxygen transport in LaCoO₃: the effect of Co³⁺ magnetic states. Journal of Materials Chemistry A, 2014, 2, 8060-8074.	10.3	76
12	First-principles study of Na insertion at TiO₂ anatase surfaces: new hints for Na-ion battery design. Nanoscale Advances, 2020, 2, 2745-2751.	4.6	75
13	Structural, electronic, and spectroscopic effects of Ga codoping on Ce-doped yttrium aluminum garnet: First-principles study. Physical Review B, 2010, 82, .	3.2	70
14	Theoretical Investigation of H₂ Oxidation on the Sr₂Fe_{1.5}Mo_{0.5}O₆ (001) Perovskite Surface under Anodic Solid Oxide Fuel Cell Conditions. Journal of the American Chemical Society, 2014, 136, 8374-8386.	13.7	68
15	Tuning optical and electronic properties in novel carbazole photosensitizers for p-type dye-sensitized solar cells. Electrochimica Acta, 2018, 292, 805-816.	5.2	67
16	Challenges of modeling nanostructured materials for photocatalytic water splitting. Chemical Society Reviews, 2022, 51, 3794-3818.	38.1	64
17	Oxide ion transport in Sr2Fe1.5Mo0.5O6â^Î´, a mixed ion-electron conductor: new insights from first principles modeling. Physical Chemistry Chemical Physics, 2013, 15, 6250.	2.8	59
18	Computational design of cobalt-free mixed protonâ€“electron conductors for solid oxide electrochemical cells. Journal of Materials Chemistry A, 2017, 5, 11825-11833.	10.3	57

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19	Sweet graphene: exfoliation of graphite and preparation of glucose-graphene cocrystals through mechanochemical treatments. Green Chemistry, 2018, 20, 3581-3592.	9.0	56
20	Structural effects and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi><mml:mtext>â^'</mml:mtext><mml:mn>5</mml:mn><mml:r shifts induced by La codoping in Ce-doped yttrium aluminum garnet: First-principles study. Physical Review B, 2010, 82, .	3.2	54
21	Effect of Coordination Sphere Geometry of Copper Redox Mediators on Regeneration and Recombination Behavior in Dye-Sensitized Solar Cell Applications. ACS Applied Energy Materials, 2018, 1, 4950-4962.	5.1	49
22	Solidâ€State Post Li Metal Ion Batteries: A Sustainable Forthcoming Reality?. Advanced Energy Materials, 2021, 11, .	19.5	49
23	Non-innocent Dissociation of H₂O on GaP(110): Implications for Electrochemical Reduction of CO₂. Journal of the American Chemical Society, 2012, 134, 13600-13603.	13.7	48
24	Ce and La Single- and Double-Substitutional Defects in Yttrium Aluminum Garnet: First-Principles Study. Journal of Physical Chemistry A, 2011, 115, 815-823.	2.5	46
25	Atomistic and electronic structure of antisite defects in yttrium aluminum garnet: Density-functional study. Physical Review B, 2009, 80, .	3.2	45
26	Luminescent solar concentrators based on PMMA films obtained from a red-emitting ATRP initiator. Polymer Chemistry, 2018, 9, 1168-1177.	3.9	43
27	Firstâ€principles study of the structure and the electronic structure of yttrium aluminum garnet Y₃Al₅O₁₂. International Journal of Quantum Chemistry, 2009, 109, 1991-1998.	2.0	40
28	Origin and Electronic Features of Reactive Oxygen Species at Hybrid Zirconia-Acetylacetonate Interfaces. ACS Applied Materials & Interfaces, 2015, 7, 21662-21667.	8.0	39
29	Antisite defects in Ce-doped YAG (Y3Al5O12): first-principles study on structures and 4fâ€“5d transitions. Journal of Materials Chemistry, 2012, 22, 19888.	6.7	38
30	Structure and energy level alignment at the dyeâ€“electrode interface in p-type DSSCs: new hints on the role of anchoring modes from ab initio calculations. Physical Chemistry Chemical Physics, 2015, 17, 12238-12246.	2.8	38
31	Experimental and Theoretical Investigation on the Catalytic Generation of Environmentally Persistent Free Radicals from Benzene. Journal of Physical Chemistry C, 2017, 121, 9381-9393.	3.1	38
32	Copper Complexes with Tetradentate Ligands for Enhanced Charge Transport in Dye-Sensitized Solar Cells. Inorganics, 2018, 6, 53.	2.7	36
33	Cost-effective solar concentrators based on red fluorescent Zn(<scp>ii</scp>)â€“salicylaldiminato complex. RSC Advances, 2016, 6, 17474-17482.	3.6	34
34	Unveiling Oxygen Redox Activity in P2-Type Na_xNi_{0.25}Mn_{0.68}O₂ High-Energy Cathode for Na-Ion Batteries. ACS Energy Letters, 2021, 6, 2470-2480.	17.4	32
35	Cluster Models for Studying CO2 Reduction on Semiconductor Photoelectrodes. Topics in Catalysis, 2015, 58, 46-56.	2.8	30
36	In Situ Formation of Zwitterionic Ligands: Changing the Passivation Paradigms of CsPbBr₃ Nanocrystals. Nano Letters, 2022, 22, 4437-4444.	9.1	30

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37	Role of surface defects in CO2 adsorption and activation on CuFeO2 delafossite oxide. Molecular Catalysis, 2020, 496, 111181.	2.0	29
38	Revealing the Mechanism of Doping of spiro-MeOTAD via Zn Complexation in the Absence of Oxygen and Light. ACS Energy Letters, 2020, 5, 1271-1277.	17.4	29
39	Ab initio evaluation of oxygen diffusivity in LaFeO3: the role of lanthanum vacancies. MRS Communications, 2013, 3, 161-166.	1.8	26
40	An ab initio study of Cu-based delafossites as an alternative to nickel oxide in photocathodes: effects of Mg-doping and surface electronic features. Physical Chemistry Chemical Physics, 2018, 20, 14082-14089.	2.8	26
41	H₂-Evolving Dye-Sensitized Photocathode Based on a Rutheniumâ€“Diacetylide/Cobaloxime Supramolecular Assembly. ACS Applied Energy Materials, 2019, 2, 4971-4980.	5.1	26
42	Analysis of the Phase Stability of LiMO2 Layered Oxides (M = Co, Mn, Ni). Crystals, 2020, 10, 526.	2.2	23
43	First-Principles Study of Na Intercalation and Diffusion Mechanisms at 2D MoS₂/Graphene Interfaces. Journal of Physical Chemistry C, 2021, 125, 2276-2286.	3.1	23
44	Design and synthesis of novel organometallic dyes for NiO sensitization and photo-electrochemical applications. Dalton Transactions, 2016, 45, 12539-12547.	3.3	21
45	K-doped Sr₂Fe_{1.5}Mo_{0.5}O_{6â^'Î´} predicted as a bifunctional catalyst for air electrodes in proton-conducting solid oxide electrochemical cells. Journal of Materials Chemistry A, 2017, 5, 12735-12739.	10.3	21
46	Simple Ethanol Refluxing Method for Production of Blue-Colored Titanium Dioxide with Oxygen Vacancies and Visible Light-Driven Photocatalytic Properties. Journal of Physical Chemistry C, 2020, 124, 3564-3576.	3.1	21
47	Monoclinic and Orthorhombic NaMnO2 for Secondary Batteries: A Comparative Study. Energies, 2021, 14, 1230.	3.1	19
48	Investigating Light-Driven Hole Injection and Hydrogen Evolution Catalysis at Dye-Sensitized NiO Photocathodes: A Combined Experimentalâ€“Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 17176-17184.	3.1	18
49	Nanometric Fe-Substituted ZrO₂on Carbon Black as PGM-Free ORR Catalyst for PEMFCs. Journal of the Electrochemical Society, 2019, 166, F3032-F3043.	2.9	18
50	Promoting oxygen vacancy formation and p-type conductivity in SrTiO₃via alkali metal doping: a first principles study. Physical Chemistry Chemical Physics, 2016, 18, 28951-28959.	2.8	17
51	Stability of melamine-exfoliated graphene in aqueous media: quantum-mechanical insights at the nanoscale. Physical Chemistry Chemical Physics, 2016, 18, 22203-22209.	2.8	16
52	Ab initio study of PbCr_(1â^'x)S_xO₄ solid solution: an inside look at Van Gogh Yellow degradation. Chemical Science, 2016, 7, 4197-4203.	7.4	16
53	Ab initio Study of Anchoring Groups for CuGaO2 Delafossite-Based p-Type Dye Sensitized Solar Cells. Frontiers in Chemistry, 2019, 7, 158.	3.6	15
54	From oxide to proton conduction: A quantumâ€chemical perspective on the versatility of Sr₂Fe_{1.5}Mo_{0.5}O_{6â^'Î´}â€based materials. International Journal of Quantum Chemistry, 2016, 116, 1501-1506.	2.0	13

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55	Tuning dispersion correction in DFT-D2 for metal-molecule interactions: A tailored reparameterization strategy for the adsorption of aromatic systems on Ag(1â€¯1â€¯1). Chemical Physics Letters, 2018, 693, 28-33.	2.6	13
56	Interfacial electronic features in methyl-ammonium lead iodide and p-type oxide heterostructures: new insights for inverted perovskite solar cells. Physical Chemistry Chemical Physics, 2020, 22, 28401-28413.	2.8	12
57	Structural evolution of disordered LiCo_{1/3}Fe_{1/3}Mn_{1/3}PO₄ in lithium batteries uncovered. Journal of Materials Chemistry A, 2020, 8, 19641-19653.	10.3	11
58	Oxygen evolution reaction at the Mo/W-doped bismuth vanadate surface: Assessing the dopant role by DFT calculations. Molecular Catalysis, 2022, 517, 112036.	2.0	11
59	Breaking Symmetry Rules Enhance the Options for Stereoselective Propene Polymerization Catalysis. Macromolecules, 2020, 53, 2959-2964.	4.8	10
60	d-Glucose Adsorption on the TiO2 Anatase (100) Surface: A Direct Comparison Between Cluster-Based and Periodic Approaches. Frontiers in Chemistry, 2021, 9, 716329.	3.6	9
61	Colourless luminescent solar concentrators based on Iridium(III)-Phosphors. Dyes and Pigments, 2021, 193, 109532.	3.7	9
62	Orbital-Resolved Imaging of the Adsorbed State of Pyridine on GaP(110) Identifies Sites Susceptible to Nucleophilic Attack. Journal of Physical Chemistry C, 2015, 119, 28917-28924.	3.1	8
63	Confinement of Semiconductor ZnO Nanoparticles in Block Copolymer Nanostructure. Journal of Physical Chemistry C, 2017, 121, 16617-16628.	3.1	8
64	Investigating Light-Induced Processes in Covalent Dye-Catalyst Assemblies for Hydrogen Production. Catalysts, 2020, 10, 1340.	3.5	8
65	Structural and electronic properties of defective 2D transition metal dichalcogenide heterostructures. Journal of Computational Chemistry, 2020, 41, 1946-1955.	3.3	8
66	First-principles study of trimethylamine adsorption on anatase TiO2 nanorod surfaces. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	7
67	Effective scheme for partitioning covalent bonds in density-functional embedding theory: From molecules to extended covalent systems. Journal of Chemical Physics, 2016, 145, 244103.	3.0	6
68	A fast route for the synthesis of tetrazolyl oximes by a novel multicomponent reaction between Z-chlorooximes, isocyanides and trimethylsilyl azide. Tetrahedron Letters, 2017, 58, 3549-3553.	1.4	6
69	Na uptake at TiO2 anatase surfaces under electric field control: A first-principles study. Journal of Materials Research, 2022, 37, 3216-3226.	2.6	6
70	Firstâ€principles insights on anion redox activity in Na_xFe_{1/8}Ni_{1/8}Mn_{3/4}O₂: Toward efficient highâ€energy cathodes for Naâ€ion batteries. Journal of the American Ceramic Society, 2023, 106, 109-119.	3.8	5
71	Unexpected Imidazole Coordination to the Dirhodium Center in a Protein Environment: Insights from X-ray Crystallography and Quantum Chemistry. Inorganic Chemistry, 2022, 61, 8402-8405.	4.0	5
72	Tuning perovskiteâ€“based oxides for effective electrodes in solid oxide electrochemical cells. , 2020, , 1-25.		4

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73	Molecular adsorption of iminotriazine derivatives on graphene. JPhys Materials, 2020, 3, 034011.	4.2	4
74	Replacement of Cobalt in Lithium-Rich Layered Oxides by n-Doping: A DFT Study. Applied Sciences (Switzerland), 2021, 11, 10545.	2.5	4
75	Development of SnO2 Composites as Electron Transport Layer in Unencapsulated CH3NH3PbI3 Solar Cells. Solids, 2021, 2, 407-419.	2.4	4
76	Electronic structure and interfacial features of triphenylamine- and phenothiazine-based hole transport materials for methylammonium lead iodide perovskite solar cells. Physical Chemistry Chemical Physics, 2022, 24, 14993-15002.	2.8	4
77	NAi/Li Antisite Defects in the Li1.2Ni0.2Mn0.6O2 Li-Rich Layered Oxide: A DFT Study. Crystals, 2022, 12, 723.	2.2	3
78	Doped graphene and Ag(1â€¯1â€¯1) hybrid material as fuel cell electrode: New insights on interfacial features and oxygen adsorption from dispersion-corrected density functional theory. Computational Materials Science, 2019, 169, 109141.	3.0	2