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	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
2	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
3	Challenges of modeling nanostructured materials for photocatalytic water splitting. Chemical Society Reviews, 2022, 51, 3794-3818.	38.1	64
4	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
5	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
6	NAi/Li Antisite Defects in the Li1.2Ni0.2Mn0.6O2 Li-Rich Layered Oxide: A DFT Study. Crystals, 2022, 12, 723.	2.2	3
7	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
8	In Situ Formation of Zwitterionic Ligands: Changing the Passivation Paradigms of CsPbBr₃ Nanocrystals. Nano Letters, 2022, 22, 4437-4444.	9.1	30
9	Monoclinic and Orthorhombic NaMnO2 for Secondary Batteries: A Comparative Study. Energies, 2021, 14, 1230.	3.1	19
10	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
11	Solidâ€State Post Li Metal Ion Batteries: A Sustainable Forthcoming Reality?. Advanced Energy Materials, 2021, 11, .	19.5	49
12	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
13	Colourless luminescent solar concentrators based on Iridium(III)-Phosphors. Dyes and Pigments, 2021, 193, 109532.	3.7	9
14	Dye-sensitized solar cells strike back. Chemical Society Reviews, 2021, 50, 12450-12550.	38.1	240
15	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
16	Replacement of Cobalt in Lithium-Rich Layered Oxides by n-Doping: A DFT Study. Applied Sciences (Switzerland), 2021, 11, 10545.	2.5	4
17	Development of SnO2 Composites as Electron Transport Layer in Unencapsulated CH3NH3PbI3 Solar Cells. Solids, 2021, 2, 407-419.	2.4	4
18	Investigating Light-Induced Processes in Covalent Dye-Catalyst Assemblies for Hydrogen Production. Catalysts, 2020, 10, 1340.	3.5	8

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19	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
20	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
21	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
22	Role of surface defects in CO2 adsorption and activation on CuFeO2 delafossite oxide. Molecular Catalysis, 2020, 496, 111181.	2.0	29
23	Structural and electronic properties of defective 2D transition metal dichalcogenide heterostructures. Journal of Computational Chemistry, 2020, 41, 1946-1955.	3.3	8
24	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
25	Analysis of the Phase Stability of LiMO2 Layered Oxides (M = Co, Mn, Ni). Crystals, 2020, 10, 526.	2.2	23
26	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
27	Breaking Symmetry Rules Enhance the Options for Stereoselective Propene Polymerization Catalysis. Macromolecules, 2020, 53, 2959-2964.	4.8	10
28	Tuning perovskiteâ€“based oxides for effective electrodes in solid oxide electrochemical cells. , 2020, , 1-25.		4
29	Molecular adsorption of iminotriazine derivatives on graphene. JPhys Materials, 2020, 3, 034011.	4.2	4
30	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
31	H₂-Evolving Dye-Sensitized Photocathode Based on a Rutheniumâ€“Diacetylide/Cobaloxime Supramolecular Assembly. ACS Applied Energy Materials, 2019, 2, 4971-4980.	5.1	26
32	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
33	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
34	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
35	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
36	Luminescent solar concentrators based on PMMA films obtained from a red-emitting ATRP initiator. Polymer Chemistry, 2018, 9, 1168-1177.	3.9	43

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37	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
38	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
39	Sweet graphene: exfoliation of graphite and preparation of glucose-graphene cocrystals through mechanochemical treatments. Green Chemistry, 2018, 20, 3581-3592.	9.0	56
40	Combined Structural, Chemometric, and Electrochemical Investigation of Vertically Aligned TiO₂ Nanotubes for Na-ion Batteries. ACS Omega, 2018, 3, 8440-8450.	3.5	86
41	Copper Complexes with Tetradentate Ligands for Enhanced Charge Transport in Dye-Sensitized Solar Cells. Inorganics, 2018, 6, 53.	2.7	36
42	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
43	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
44	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
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	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
47	Confinement of Semiconductor ZnO Nanoparticles in Block Copolymer Nanostructure. Journal of Physical Chemistry C, 2017, 121, 16617-16628.	3.1	8
48	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
49	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
50	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
51	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
52	Design and synthesis of novel organometallic dyes for NiO sensitization and photo-electrochemical applications. Dalton Transactions, 2016, 45, 12539-12547.	3.3	21
53	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
54	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

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55	Cost-effective solar concentrators based on red fluorescent Zn(<scp>ii</scp>)â€“salicylaldiminato complex. RSC Advances, 2016, 6, 17474-17482.	3.6	34
56	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
57	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
58	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
59	Cluster Models for Studying CO2 Reduction on Semiconductor Photoelectrodes. Topics in Catalysis, 2015, 58, 46-56.	2.8	30
60	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
61	First-principles study of trimethylamine adsorption on anatase TiO2 nanorod surfaces. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	7
62	Origin and Electronic Features of Reactive Oxygen Species at Hybrid Zirconia-Acetylacetonate Interfaces. ACS Applied Materials & Interfaces, 2015, 7, 21662-21667.	8.0	39
63	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
64	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
65	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
66	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
67	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
68	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
69	Ab initio evaluation of oxygen diffusivity in LaFeO3: the role of lanthanum vacancies. MRS Communications, 2013, 3, 161-166.	1.8	26
70	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
71	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
72	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

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73	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
74	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
75	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
76	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:m shifts induced by La codoping in Ce-doped yttrium aluminum garnet: First-principles study. Physical Review B, 2010, 82, .	3.2	54
77	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
78	Atomistic and electronic structure of antisite defects in yttrium aluminum garnet: Density-functional study. Physical Review B, 2009, 80, .	3.2	45