Ãngel Morales GarcÃ-a

List of Publications by Year
in descending order

70	2,326	279487 23	223531 46
papers	citations	h-index	g-index

71	71	71	3085
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical calculations of the effect of nitrogen substitution on the structural, vibrational, and electronic properties of wolframite-type ScTaO₄at ambient conditions. Dalton Transactions, 2022, 51, 3642-3651.	1.6	3
2	Effect of oxygen termination on the interaction of first row transition metals with M₂C MXenes and the feasibility of single-atom catalysts. Journal of Materials Chemistry A, 2022, 10, 8846-8855.	5.2	18
3	Effect of the sulfur termination on the properties of Hf₂CO₂MXene. Physical Chemistry Chemical Physics, 2022, 24, 7243-7252.	1.3	17
4	Challenges of modeling nanostructured materials for photocatalytic water splitting. Chemical Society Reviews, 2022, 51, 3794-3818.	18.7	64
5	Understanding the thermodynamic, dynamic, bonding, and electrocatalytic properties of low-dimensional MgPSe₃. Dalton Transactions, 2022, 51, 9689-9698.	1.6	8
6	Flexibilization of Biorefineries: Tuning Lignin Hydrogenation by Hydrogen Partial Pressure. ChemSusChem, 2021, 14, 373-378.	3.6	8
7	Assigning XPS features in B,N-doped graphene: input from ab initio quantum chemical calculations. Physical Chemistry Chemical Physics, 2021, 23, 1558-1565.	1.3	8
8	Exfoliation Energy as a Descriptor of MXenes Synthesizability and Surface Chemical Activity. Nanomaterials, 2021, 11, 127.	1.9	22
9	Relating X-ray photoelectron spectroscopy data to chemical bonding in MXenes. Nanoscale Advances, 2021, 3, 2793-2801.	2.2	11
10	Interaction of First Row Transition Metals with M₂C (M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.5	38
11	Understanding the nature and location of hydroxyl groups on hydrated titania nanoparticles. Nanoscale, 2021, 13, 6577-6585.	2.8	35
12	Pressure-Driven Metallization in Hafnium Diselenide. Inorganic Chemistry, 2021, 60, 1746-1754.	1.9	8
13	Concepts, models, and methods in computational heterogeneous catalysis illustrated through <scp>CO₂</scp> conversion. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1530.	6.2	24
14	Understanding the Structural and Electronic Properties of Photoactive Tungsten Oxide Nanoparticles from Density Functional Theory and GW Approaches. Journal of Chemical Theory and Computation, 2021, 17, 3462-3470.	2.3	14
15	Carbon Capture and Usage by MXenes. ACS Catalysis, 2021, 11, 11248-11255.	5.5	40
16	Adsorption and Activation of CO₂ on Nitride MXenes: Composition, Temperature, and Pressure effects. ChemPhysChem, 2021, 22, 2456-2463.	1.0	11
17	Low-dimensional HfS₂as SO₂adsorbent and gas sensor: effect of water and sulfur vacancies. Physical Chemistry Chemical Physics, 2021, 23, 23655-23666.	1.3	7
18	Thermodynamics and Kinetics of Molecular Hydrogen Adsorption and Dissociation on MXenes: Relevance to Heterogeneously Catalyzed Hydrogenation Reactions. ACS Catalysis, 2021, 11, 12850-12857.	5.5	19

#	Article	IF	Citations
19	Tuning the Interfacial Energetics in WO₃/WO₃ and WO₃/TiO₂ Heterojunctions by Nanostructure Morphological Engineering. Journal of Physical Chemistry Letters, 2021, 12, 11528-11533.	2.1	12
20	Identifying the Atomic Layer Stacking of Mo₂C MXene by Probe Molecule Adsorption. Journal of Physical Chemistry C, 2021, 125, 26808-26813.	1.5	8
21	MXenes as promising catalysts for water dissociation. Applied Catalysis B: Environmental, 2020, 260, 118191.	10.8	94
22	Investigating the character of excited states in TiO₂nanoparticles from topological descriptors: implications for photocatalysis. Physical Chemistry Chemical Physics, 2020, 22, 3017-3029.	1.3	15
23	Bulk (in)stability as a possible source of surface reconstruction. Physical Chemistry Chemical Physics, 2020, 22, 19249-19253.	1.3	6
24	MXenes: New Horizons in Catalysis. ACS Catalysis, 2020, 10, 13487-13503.	5.5	239
25	Morphology of TiO₂ Nanoparticles as a Fingerprint for the Transient Absorption Spectra: Implications for Photocatalysis. Journal of Physical Chemistry C, 2020, 124, 11819-11824.	1.5	8
26	Structural and vibrational behavior of cubic Cu1.80(3)Se cuprous selenide, berzelianite, under compression. Journal of Alloys and Compounds, 2020, 830, 154646.	2.8	1
27	On the use of DFT+U to describe the electronic structure of TiO2 nanoparticles: (TiO2)35 as a case study. Journal of Chemical Physics, 2020, 152, 244107.	1.2	7
28	Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes. ACS Catalysis, 2020, 10, 5049-5056.	5.5	67
29	Comprehensive analysis of the influence of dispersion on group-14 rutile-type solids. Physical Review Materials, 2020, 4, .	0.9	1
30	Electronic Properties of Realistic Anatase TiO₂ Nanoparticles from G₀W₀ Calculations on a Gaussian and Plane Waves Scheme. Journal of Chemical Theory and Computation, 2019, 15, 5024-5030.	2.3	7
31	Efficient preparation of TiO2 nanoparticle models using interatomic potentials. Journal of Chemical Physics, 2019, 150, 214305.	1.2	9
32	Understanding the interplay between size, morphology and energy gap in photoactive TiO₂nanoparticles. Nanoscale, 2019, 11, 9032-9041.	2.8	45
33	Thickness biased capture of CO₂ on carbide MXenes. Physical Chemistry Chemical Physics, 2019, 21, 23136-23142.	1.3	55
34	Electronic, bonding, linear, and nonlinear optical properties of Na2MGe2Q6 (M=Cd, Zn, Hg; Q=S, Se), Na2ZnSi2S6, and Na2ZnSn2S6 two metal-mixed chalcogenide compounds: Insights from an ab initio study. Journal of Physics and Chemistry of Solids, 2018, 119, 220-227.	1.9	14
35	CO₂abatement using two-dimensional MXene carbides. Journal of Materials Chemistry A, 2018, 6, 3381-3385.	5.2	152
36	Properties of Single Oxygen Vacancies on a Realistic (TiO₂)₈₄ Nanoparticle: A Challenge for Density Functionals. Journal of Physical Chemistry C, 2018, 122, 2413-2421.	1.5	22

#	Article	IF	Citations
37	Pressure-induced chemistry for the 2D to 3D transformation of zeolites. Journal of Materials Chemistry A, 2018, 6, 5255-5259.	5.2	21
38	Two-dimensional nitrides as highly efficient potential candidates for CO₂ capture and activation. Physical Chemistry Chemical Physics, 2018, 20, 17117-17124.	1.3	55
39	Quantum-mechanical simulations of pressure effects on MgIn₂S₄ polymorphs. Phase Transitions, 2018, 91, 759-771.	0.6	6
40	Reliable and computationally affordable prediction of the energy gap of (TiO₂)_n(10 â‰¤nâ‰¤ 563) nanoparticles from density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 18907-18911.	1.3	18
41	Theoretical Modeling of Electronic Excitations of Gas-Phase and Solvated TiO₂ Nanoclusters and Nanoparticles of Interest in Photocatalysis. Journal of Chemical Theory and Computation, 2018, 14, 4391-4404.	2.3	24
42	Two-dimensional silicon carbide structure under uniaxial strains, electronic and bonding analysis. Computational Materials Science, 2018, 151, 288-295.	1.4	26
43	Fine tuning of optical transition energy of twisted bilayer graphene via interlayer distance modulation. Physical Review B, 2017, 95, .	1.1	12
44	Surfaces and morphologies of covellite (CuS) nanoparticles by means of ab initio atomistic thermodynamics. CrystEngComm, 2017, 19, 3078-3084.	1.3	38
45	Tuning the electronic properties of monolayer and bilayer transition metal dichalcogenide compounds under direct out-of-plane compression. Physical Chemistry Chemical Physics, 2017, 19, 13333-13340.	1.3	20
46	The Influence of Water on the Performance of Molybdenum Carbide Catalysts in Hydrodeoxygenation Reactions: A Combined Theoretical and Experimental Study. ChemCatChem, 2017, 9, 1985-1991.	1.8	29
47	Two-dimensional crystal CuSâ€"electronic and structural properties. 2D Materials, 2017, 4, 015041.	2.0	20
48	Exploring the stability and reactivity of Ni2P and Mo2C catalysts using ab initio atomistic thermodynamics and conceptual DFT approaches. Biomass Conversion and Biorefinery, 2017, 7, 377-383.	2.9	3
49	An Empirical, yet Practical Way To Predict the Band Gap in Solids by Using Density Functional Band Structure Calculations. Journal of Physical Chemistry C, 2017, 121, 18862-18866.	1.5	165
50	Performance of theG₀W₀Method in Predicting the Electronic Gap of TiO₂Nanoparticles. Journal of Chemical Theory and Computation, 2017, 13, 3746-3753.	2.3	20
51	The interaction of Pd clusters with the bulk and layered two-dimensional Silicalite-1 supports. Catalysis Today, 2016, 277, 108-117.	2.2	2
52	The surface stability and equilibrium crystal morphology of Ni₂P nanoparticles and nanowires from an ab initio atomistic thermodynamic approach. CrystEngComm, 2016, 18, 3808-3818.	1.3	17
53	The Stability and Structural, Electronic and Topological Properties of Covellite (001) Surfaces.. ChemistrySelect, 2016, 1, 2730-2741.	0.7	15
54	High temperature spin-polarized semiconductivity with zero magnetization in two-dimensional Janus MXenes. Journal of Materials Chemistry C, 2016, 4, 6500-6509.	2.7	127

#	Article	IF	Citations
55	Computer simulations of 3C-SiC under hydrostatic and non-hydrostatic stresses. Physical Chemistry Chemical Physics, 2016, 18, 8132-8139.	1.3	23
56	Combining experiments and computations to understand the intercalation potential and redox mechanism for A2Ti3O7 (A=Li, Na). Materials Research Society Symposia Proceedings, 2015, 1740, 31.	0.1	1
57	Single Layer Molybdenum Disulfide under Direct Out-of-Plane Compression: Low-Stress Band-Gap Engineering. Nano Letters, 2015, 15, 3139-3146.	4.5	75
58	A novel crystalline SiCO compound. Physical Chemistry Chemical Physics, 2015, 17, 25055-25060.	1.3	7
59	Taking steps forward in understanding the electrochemical behavior of Na₂Ti₃O₇. Journal of Materials Chemistry A, 2015, 3, 22280-22286.	5.2	51
60	Revealing the local properties ofÎ²-HP₄N₇, a promising candidate for high pressure synthesis of new materials. Materials Research Express, 2015, 2, 045904.	0.8	0
61	From micro-to macroscopic: Understanding optical properties in zinc-blend-derived materials Cu2ZnYX4(XÂ=ÂS, Se, Te, YÂ=ÂSi, Ge, Sn) by means of the quantum chemical topology analysis. Journal of Alloys and Compounds, 2015, 653, 140-147.	2.8	8
62	A local topological view of pressure-induced polymorphs in SiO2. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	6
63	Pbca-Type In₂O₃: The High-Pressure Post-Corundum phase at Room Temperature.. Journal of Physical Chemistry C, 2014, 118, 20545-20552.	1.5	27
64	First-Principles Calculations and Electron Density Topological Analysis of Covellite (CuS). Journal of Physical Chemistry A, 2014, 118, 5823-5831.	1.1	111
65	Preparation, Crystal Structure, and Magnetotransport Properties of the New CdCu₃Mn₄O₁₂ Perovskite: A Comparison with Density Functional Theory Calculations. Journal of Physical Chemistry C, 2014, 118, 9652-9658.	1.5	9
66	First-principles study of structure and stability in Siâ€“Câ€“O-based materials. Highlights in Theoretical Chemistry, 2014, , 197-201.	0.0	0
67	First-principles study of structure and stability in Siâ€“Câ€“O-based materials. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	8
68	Understanding Chemical Changes across the Î±-Cristobalite to Stishovite Transition Path in Silica. Journal of Physical Chemistry C, 2013, 117, 8950-8958.	1.5	15
69	Structural Phase Transitions on AgCuS Stromeyerite Mineral under Compression. Inorganic Chemistry, 2013, 52, 355-361.	1.9	26
70	DFT+U calculations of crystal lattice, electronic structure, and phase stability under pressure of TiO2 polymorphs. Journal of Chemical Physics, 2011, 135, 054503.	1.2	221