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	MXenes: New Horizons in Catalysis. ACS Catalysis, 2020, 10, 13487-13503.	5.5	239
2	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
3	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
4	CO₂abatement using two-dimensional MXene carbides. Journal of Materials Chemistry A, 2018, 6, 3381-3385.	5.2	152
5	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
6	First-Principles Calculations and Electron Density Topological Analysis of Covellite (CuS). Journal of Physical Chemistry A, 2014, 118, 5823-5831.	1.1	111
7	MXenes as promising catalysts for water dissociation. Applied Catalysis B: Environmental, 2020, 260, 118191.	10.8	94
8	Single Layer Molybdenum Disulfide under Direct Out-of-Plane Compression: Low-Stress Band-Gap Engineering. Nano Letters, 2015, 15, 3139-3146.	4.5	75
9	Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes. ACS Catalysis, 2020, 10, 5049-5056.	5.5	67
10	Challenges of modeling nanostructured materials for photocatalytic water splitting. Chemical Society Reviews, 2022, 51, 3794-3818.	18.7	64
11	Two-dimensional nitrides as highly efficient potential candidates for CO₂ capture and activation. Physical Chemistry Chemical Physics, 2018, 20, 17117-17124.	1.3	55
12	Thickness biased capture of CO₂ on carbide MXenes. Physical Chemistry Chemical Physics, 2019, 21, 23136-23142.	1.3	55
13	Taking steps forward in understanding the electrochemical behavior of Na₂Ti₃O₇. Journal of Materials Chemistry A, 2015, 3, 22280-22286.	5.2	51
14	Understanding the interplay between size, morphology and energy gap in photoactive TiO₂nanoparticles. Nanoscale, 2019, 11, 9032-9041.	2.8	45
15	Carbon Capture and Usage by MXenes. ACS Catalysis, 2021, 11, 11248-11255.	5.5	40
16	Surfaces and morphologies of covellite (CuS) nanoparticles by means of ab initio atomistic thermodynamics. CrystEngComm, 2017, 19, 3078-3084.	1.3	38
17	Interaction of First Row Transition Metals with M₂C (M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	38
18	Understanding the nature and location of hydroxyl groups on hydrated titania nanoparticles. Nanoscale, 2021, 13, 6577-6585.	2.8	35

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19	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
20	Pbca-Type In₂O₃: The High-Pressure Post-Corundum phase at Room Temperature.. Journal of Physical Chemistry C, 2014, 118, 20545-20552.	1.5	27
21	Structural Phase Transitions on AgCuS Stromeyerite Mineral under Compression. Inorganic Chemistry, 2013, 52, 355-361.	1.9	26
22	Two-dimensional silicon carbide structure under uniaxial strains, electronic and bonding analysis. Computational Materials Science, 2018, 151, 288-295.	1.4	26
23	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
24	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
25	Computer simulations of 3C-SiC under hydrostatic and non-hydrostatic stresses. Physical Chemistry Chemical Physics, 2016, 18, 8132-8139.	1.3	23
26	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
27	Exfoliation Energy as a Descriptor of MXenes Synthesizability and Surface Chemical Activity. Nanomaterials, 2021, 11, 127.	1.9	22
28	Pressure-induced chemistry for the 2D to 3D transformation of zeolites. Journal of Materials Chemistry A, 2018, 6, 5255-5259.	5.2	21
29	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
30	Two-dimensional crystal CuSâ€"electronic and structural properties. 2D Materials, 2017, 4, 015041.	2.0	20
31	Performance of theG₀W₀Method in Predicting the Electronic Gap of TiO₂Nanoparticles. Journal of Chemical Theory and Computation, 2017, 13, 3746-3753.	2.3	20
32	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
33	Reliable and computationally affordable prediction of the energy gap of (TiO₂)_n (10 â‰¤ n â‰¤ 563) nanoparticles from density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 18907-18911.	1.3	18
34	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
35	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
36	Effect of the sulfur termination on the properties of Hf₂CO₂MXene. Physical Chemistry Chemical Physics, 2022, 24, 7243-7252.	1.3	17

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37	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
38	The Stability and Structural, Electronic and Topological Properties of Covellite (001) Surfaces.. ChemistrySelect, 2016, 1, 2730-2741.	0.7	15
39	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
40	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
41	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
42	Fine tuning of optical transition energy of twisted bilayer graphene via interlayer distance modulation. Physical Review B, 2017, 95, .	1.1	12
43	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
44	Relating X-ray photoelectron spectroscopy data to chemical bonding in MXenes. Nanoscale Advances, 2021, 3, 2793-2801.	2.2	11
45	Adsorption and Activation of CO₂ on Nitride MXenes: Composition, Temperature, and Pressure effects. ChemPhysChem, 2021, 22, 2456-2463.	1.0	11
46	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
47	Efficient preparation of TiO2 nanoparticle models using interatomic potentials. Journal of Chemical Physics, 2019, 150, 214305.	1.2	9
48	First-principles study of structure and stability in Siâ€“Câ€“O-based materials. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	8
49	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
50	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
51	Flexibilization of Biorefineries: Tuning Lignin Hydrogenation by Hydrogen Partial Pressure. ChemSusChem, 2021, 14, 373-378.	3.6	8
52	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
53	Pressure-Driven Metallization in Hafnium Diselenide. Inorganic Chemistry, 2021, 60, 1746-1754.	1.9	8
54	Identifying the Atomic Layer Stacking of Mo₂C MXene by Probe Molecule Adsorption. Journal of Physical Chemistry C, 2021, 125, 26808-26813.	1.5	8

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55	Understanding the thermodynamic, dynamic, bonding, and electrocatalytic properties of low-dimensional MgPSe₃. Dalton Transactions, 2022, 51, 9689-9698.	1.6	8
56	A novel crystalline SiCO compound. Physical Chemistry Chemical Physics, 2015, 17, 25055-25060.	1.3	7
57	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
58	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
59	Low-dimensional HfS₂as SO₂adsorbent and gas sensor: effect of water and sulfur vacancies. Physical Chemistry Chemical Physics, 2021, 23, 23655-23666.	1.3	7
60	A local topological view of pressure-induced polymorphs in SiO2. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	6
61	Quantum-mechanical simulations of pressure effects on MgIn₂S₄ polymorphs. Phase Transitions, 2018, 91, 759-771.	0.6	6
62	Bulk (in)stability as a possible source of surface reconstruction. Physical Chemistry Chemical Physics, 2020, 22, 19249-19253.	1.3	6
63	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
64	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
65	The interaction of Pd clusters with the bulk and layered two-dimensional Silicalite-1 supports. Catalysis Today, 2016, 277, 108-117.	2.2	2
66	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
67	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
68	Comprehensive analysis of the influence of dispersion on group-14 rutile-type solids. Physical Review Materials, 2020, 4, .	0.9	1
69	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
70	First-principles study of structure and stability in Siâ€“Câ€“O-based materials. Highlights in Theoretical Chemistry, 2014, , 197-201.	0.0	0