Antonio M MÃ¡rquez

List of Publications by Year
in descending order

84 papers	2,252 citations	201674 27 h-index	243625 44 g-index
89 all docs	89 docs citations	89 times ranked	2852 citing authors

#	Article	IF	Citations
1	Catalytic activity of PtCu intermetallic compound for CO oxidation: A theoretical insight. Catalysis Today, 2022, 383, 339-344.	4.4	2
2	Optoelectronic properties of Ag2S/graphene and FeS2/graphene nanostructures and interfaces: A density functional study including dispersion forces. Journal of Materials Research, 2022, 37, 1047-1058.	2.6	2
3	Charting the Lattice Thermal Conductivities of Iâ€“IIIâ€“VI₂ Chalcopyrite Semiconductors. Chemistry of Materials, 2022, 34, 2833-2841.	6.7	22
4	Connecting experimental synthetic variables with the microstructure and electronic properties of doped ferroelectric perovskites for solar cell applications using high-throughput frameworks. Acta Materialia, 2021, 204, 116466.	7.9	4
5	High-Throughput Screening of the Thermoelastic Properties of Ultrahigh-Temperature Ceramics. ACS Applied Materials & Interfaces, 2021, 13, 29843-29857.	8.0	8
6	Comprehensive Experimental and Theoretical Study of the CO + NO Reaction Catalyzed by Au/Ni Nanoparticles. ACS Catalysis, 2019, 9, 4919-4929.	11.2	22
7	Understanding the Photocatalytic Properties of Pt/CeO_x/TiO₂: Structural Effects on Electronic and Optical Properties. ChemPhysChem, 2019, 20, 1624-1629.	2.1	8
8	Photo-sensitizing thin-film ferroelectric oxides using materials databases and high-throughput calculations. Journal of Materials Chemistry A, 2019, 7, 27323-27333.	10.3	12
9	Adsorption of Prototypical Asphaltenes on Silica: First-Principles DFT Simulations Including Dispersion Corrections. Journal of Physical Chemistry B, 2018, 122, 618-624.	2.6	21
10	Analysis of the variables that modify the robustness of Ti-SiO2 catalysts for alkene epoxidation: Role of silylation, deactivation and potential solutions. Molecular Catalysis, 2018, 459, 55-60.	2.0	9
11	Improving the activity of gold nanoparticles for the water-gas shift reaction using TiO₂â€“Y₂O₃: an example of catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 22076-22083.	2.8	8
12	Structural and electronic properties of lead sulfide quantum dots from screened hybrid density functional calculations including spinâ€“orbit coupling effects. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	3
13	Effects of the capping ligands, linkers and oxide surface on the electron injection mechanism of copper sulfide quantum dot-sensitized solar cells. Physical Chemistry Chemical Physics, 2017, 19, 14580-14587.	2.8	12
14	Molecular dynamics simulations of the role of salinity and temperature on the hydrocarbon/water interfacial tension. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	16
15	Critical Role of Oxygen in Silver-Catalyzed Glaserâ€“Hay Coupling on Ag(100) under Vacuum and in Solution on Ag Particles. ACS Catalysis, 2017, 7, 3113-3120.	11.2	8
16	Host-guest interactions between cyclodextrins and surfactants with functional groups at the end of the hydrophobic tail. Journal of Colloid and Interface Science, 2017, 491, 336-348.	9.4	19
17	Ag₂S Quantum Dot-Sensitized Solar Cells by First Principles: The Effect of Capping Ligands and Linkers. Journal of Physical Chemistry A, 2017, 121, 7290-7296.	2.5	17
18	Structural, electronic and optical properties of copper, silver and gold sulfide: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	35

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19	Adsorption of prototypical amino acids on silica: Influence of the pre-adsorbed water multilayer. Surface Science, 2016, 646, 239-246.	1.9	10
20	Surface oxygen vacancies in gold based catalysts for CO oxidation. RSC Advances, 2014, 4, 13145-13152.	3.6	24
21	Understanding the Interplay of Dopants, Interfaces, and Anionic Conductivity in Doped Ceria/Zirconia Heteroepitaxial Structures. Chemistry of Materials, 2014, 26, 3385-3390.	6.7	16
22	Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Highlights in Theoretical Chemistry, 2014, , 177-183.	0.0	0
23	Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	5
24	Electron Mobility via Polaron Hopping in Bulk Ceria: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 14502-14509.	3.1	75
25	Nanosized CoO Films on the Î±-Al₂O₃ (0001) Surface: A Density Functional Study. Journal of Physical Chemistry C, 2013, 117, 22714-22722.	3.1	6
26	Transport Properties in the CeO_{2â€“x}(111) Surface: From Charge Distribution to Ion-Electron Collaborative Migration. Journal of Physical Chemistry C, 2013, 117, 25497-25503.	3.1	41
27	Making Photo-selective TiO₂ Materials by Cationâ€“Anion Codoping: From Structure and Electronic Properties to Photoactivity. Journal of Physical Chemistry C, 2012, 116, 18759-18767.	3.1	29
28	Ceria(100) Nanotubes with Negative Strain Energy: A First-Principles Prediction. Journal of Physical Chemistry Letters, 2012, 3, 2092-2096.	4.6	5
29	Communication: Improving the density functional theory+U description of CeO2 by including the contribution of the O 2p electrons. Journal of Chemical Physics, 2012, 136, 041101.	3.0	62
30	Understanding Acetaldehyde Thermal Chemistry on the TiO₂ (110) Rutile Surface: From Adsorption to Reactivity. Journal of Physical Chemistry C, 2011, 115, 2819-2825.	3.1	22
31	Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO₂and Ce₂O₃. Journal of Chemical Theory and Computation, 2011, 7, 56-65.	5.3	125
32	Structural Defects in W-Doped TiO₂ (101) Anatase Surface: Density Functional Study. Journal of Physical Chemistry C, 2011, 115, 16970-16976.	3.1	34
33	Electronic structure and optical spectra of catechol on TiO₂nanoparticles from real time TD-DFT simulations. Physical Chemistry Chemical Physics, 2011, 13, 1506-1514.	2.8	103
34	Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity. Topics in Catalysis, 2011, 54, 219-228.	2.8	25
35	Charge state of metal atoms on oxide supports: a systematic study based on simulated infrared spectroscopy and density functional theory. Theoretical Chemistry Accounts, 2010, 126, 265-273.	1.4	17
36	A Density Functional Study of Initial Steps in the Oxidation of Early Transition Metal Nitrides, MN (M =) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.1	12

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37	Role of Coverage and Surface Oxidation Degree in the Adsorption of Acetone on TiO₂(110). A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 19973-19980.	3.1	24
38	Adsorption of Pd Atoms and Dimers on the TiO2(110) Surface:â€‰ A First Principles Study. Journal of Physical Chemistry C, 2007, 111, 3949-3955.	3.1	51
39	Structure and Dynamics of Methyl-substituted Beryllocene: [Be(C5Me5)2]. Theoretical Chemistry Accounts, 2006, 116, 480-485.	1.4	6
40	Cu, Ag and Au atoms deposited on the Î±-Al2O3(0001) surface: a comparative density functional study. Surface Science, 2005, 575, 189-196.	1.9	63
41	A CSOV study of the difference between HF and DFT intermolecular interaction energy values: The importance of the charge transfer contribution. Journal of Computational Chemistry, 2005, 26, 1052-1062.	3.3	99
42	Role of vacancies in the structural stability ofÎ±â^'TiO: A first-principles study based on density-functional calculations. Physical Review B, 2005, 72, .	3.2	50
43	Adsorption of Pd atoms on Î³-Al2O3: a density functional study of metalâ€“support interactions. Applied Surface Science, 2004, 238, 82-85.	6.1	23
44	Density Functional Theory Study of Co, Rh, and Ir Atoms Deposited on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2004, 108, 15671-15678.	2.6	30
45	Synthesis, Solid-State Structure, and Bonding Analysis of the Beryllocenes[Be(C5Me4H)2],[Be(C5Me5)2], and[Be(C5Me5)(C5Me4H)]. Chemistry - A European Journal, 2003, 9, 4452-4461.	3.3	37
46	Theoretical enthalpy of formation of the acetonyl radical. Chemical Physics Letters, 2003, 373, 350-356.	2.6	17
47	Modeling of Copper(II) Complexes with the SIBFA Polarizable Molecular Mechanics Procedure. Application to a New Class of HIV-1 Protease Inhibitors. Journal of Physical Chemistry B, 2003, 107, 10640-10652.	2.6	35
48	The Effect of Pyrimidine Bases on the Hole-Transfer Coupling in DNAâ€. Journal of Physical Chemistry B, 2002, 106, 7919-7926.	2.6	24
49	The Rys quadrature revisited: A novel formulation for the efficient computation of electron repulsion integrals over Gaussian functions. Journal of Chemical Physics, 2001, 114, 2067-2078.	3.0	35
50	DFTversus CI determination of the electron-transfer matrix element in some case examples. International Journal of Quantum Chemistry, 2000, 76, 458-463.	2.0	12
51	A first principles study of Pd deposition on the TiO 2 (1 1 0) surface. Theoretical Chemistry Accounts, 2000, 104, 317-322.	1.4	11
52	Theoretical investigations of NMR chemical shieldings on the AlPON catalyst system. Journal of Non-Crystalline Solids, 2000, 263-264, 189-194.	3.1	7
53	A DFT Theoretical Analysis of Aldehyde Condensation Pathways onto Methyllithium, Lithium Dimethylamide, and Their Aggregates. Journal of Organic Chemistry, 2000, 65, 8899-8907.	3.2	45
54	Adsorption of Acetone onto MgO: Experimental and Theoretical Evidence for the Presence of a Surface Enolate. Angewandte Chemie - International Edition, 1999, 38, 506-509.	13.8	24

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55	Analysis of electronic contributions to the vibrational frequency of CO/Cu2O(111). Surface Science, 1999, 430, 137-145.	1.9	28
56	Similarities and differences in the Hartreeâ€“Fock and density-functional description of the chemisorption bond. Surface Science, 1999, 442, 463-476.	1.9	37
57	The Short-Range Structure of Aluminophosphate Oxynitride Catalysts. An ab Initio and Experimental Study. Journal of Physical Chemistry B, 1999, 103, 10850-10857.	2.6	1
58	Theoretical models for ?-Al2O3 (110) surface hydroxylation: An ab initio embedded cluster study. International Journal of Quantum Chemistry, 1998, 70, 359-365.	2.0	20
59	Optical Absorption and Nonradiative Decay Mechanism ofEâ€²Center in Silica. Physical Review Letters, 1998, 81, 377-380.	7.8	113
60	Geometric and Electronic Structure of Amorphous Aluminophosphates. Ab Initio and Experimental Studies. Journal of Physical Chemistry B, 1997, 101, 9510-9516.	2.6	18
61	On the bonding mechanism of CO to Pt(111) and its effect on the vibrational frequency of chemisorbed CO. Surface Science, 1997, 376, 279-296.	1.9	61
62	An ab initio study of the CH2O adsorption on the MgO (100) surface. Effects of replacing the active Mg2+ ion by different metallic cations. Computational and Theoretical Chemistry, 1997, 390, 177-181.	1.5	2
63	Structure of a mononuclear Rhenium catalyst supported on MgO: An ab initio study. Journal of Molecular Catalysis A, 1997, 119, 195-200.	4.8	0
64	Parallel computation of second derivatives of RHF energy on distributed memory computers. Journal of Computational Chemistry, 1997, 18, 159-168.	3.3	15
65	Importance of Madelung potential in quantum chemical modeling of ionic surfaces. Journal of Computational Chemistry, 1997, 18, 617-628.	3.3	85
66	A Theoretical Study of ZnCH2 and ZnSnH2 Electronic Structure and the ZnCH2â˜HZnCH Photolytic Rearrangement. Journal of the American Chemical Society, 1996, 118, 429-436.	13.7	9
67	Theoretical values of the enthalpies of formation of the NHx (x = 1,2,3) compounds. Importance of the core-correlation effects. Chemical Physics Letters, 1995, 233, 220-226.	2.6	20
68	Parallel computation of the MP2 energy on distributed memory computers. Journal of Computational Chemistry, 1995, 16, 395-404.	3.3	29
69	A theoretical approach to the molecular structure of vinylstannane and some structural isomers. Journal of Organometallic Chemistry, 1995, 486, 45-50.	1.8	3
70	Ab Initio SCF-Mo Study of the Chemisorption of Methane on Al and La Oxide Surfaces. Journal of Catalysis, 1995, 156, 273-278.	6.2	14
71	Origin of the vibrational shift of CO chemisorbed on Pt(111). Physical Review B, 1995, 52, 12372-12379.	3.2	65
72	On modelling the interaction of CO on the MgO(100) surface. Surface Science, 1995, 327, 59-73.	1.9	96

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73	Spectroscopic properties and potential energy curves of some low-lying electronic states of AlO, AlO+, LaO, and LaO+: An ab initioCASSCFstudy. International Journal of Quantum Chemistry, 1994, 52, 1329-1338.	2.0	33
74	An ab initio CASSCF study of the hydroxyl + nitrosyl chloride reaction. The Journal of Physical Chemistry, 1992, 96, 2115-2118.	2.9	2
75	Electronic structure of the transition-metal-carbene-like complexes (CO)5Mo-M'H2 (M' = carbon,) Tj ETQq1 1 0.784314 rgBT /Overloc American Chemical Society, 1992, 114, 2903-2909.	13.7	46
76	The vacuum-ultraviolet spectrum of iron pentacarbonyl: An experimental analysis supported by a CASSCF CCI study of the Rydberg states. The Journal of Physical Chemistry, 1992, 96, 121-123.	2.9	22
77	Valence contrast by synchrotron resonance scattering: application to a mixed-valence manganese compound. Journal of the American Chemical Society, 1992, 114, 9214-9215.	13.7	28
78	Ab initio CASSCF study of the electronic structure of the transition-metal alkylidene-like complexes Mo-M'H2 (M' = carbon, silicon, germanium and tin). Journal of the American Chemical Society, 1992, 114, 10019-10024.	13.7	20
79	The vacuum ultraviolet spectrum of [Mn2(CO)10]. Journal of Organometallic Chemistry, 1992, 434, 235-240.	1.8	7
80	Ab initio calculations of molecular and electronic structure of disilane. II. Photoelectron and vacuum UV electronic spectra. Chemical Physics, 1991, 149, 333-339.	1.9	6
81	Ab initio calculations of molecular and electronic structure of disilane. I. Molecular force field and vibrational spectrum. Chemical Physics, 1991, 149, 311-318.	1.9	11
82	Ab initio CI calculations on the molecular structure of Sn2H4 isomers. Chemical Physics, 1989, 138, 99-104.	1.9	18
83	Vibrational spectra of stannane: Harmonic force field, Raman and IR intensities from ab initio correlated wavefunctions. Chemical Physics, 1989, 130, 451-456.	1.9	3
84	Molecular structure and vibrational analysis of distannane from ab initio second-order perturbation calculations: a theoretical approach to the tin-X bond (X = C, Si, Ge, Sn). The Journal of Physical Chemistry, 1989, 93, 7328-7333.	2.9	7