Francesc Illas Riera

List of Publications by Citations

653 papers	26,317 citations	77 h-index	124 g-index
695 ext. papers	28,527 ext. citations	5.2 avg, IF	7.34 L-index

#	Paper	IF	Citations
653	Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. *Nature Materials*, **2011**, 10, 310-5	27	635
652	First-principles LDA+U and GGA+U study of cerium oxides: Dependence on the effective U parameter. *Physical Review B*, **2007**, 75,	3.3	569
651	A new type of strong metal-support interaction and the production of H2 through the transformation of water on Pt/CeO2(111) and Pt/CeO(x)/TiO2(110) catalysts. *Journal of the American Chemical Society*, **2012**, 134, 8968-74	16.4	536
650	Origin of the Large N 1s Binding Energy in X-ray Photoelectron Spectra of Calcined Carbonaceous Materials. *Journal of the American Chemical Society*, **1996**, 118, 8071-8076	16.4	441
649	A Molecular mechanism for the chemoselective hydrogenation of substituted nitroaromatics with nanoparticles of gold on TiO2 catalysts: a cooperative effect between gold and the support. *Journal of the American Chemical Society*, **2007**, 129, 16230-7	16.4	404
648	Remarks on the Proper Use of the Broken Symmetry Approach to Magnetic Coupling. *Journal of Physical Chemistry A*, **1997**, 101, 7860-7866	2.8	396
647	Effect of Fock exchange on the electronic structure and magnetic coupling in NiO. *Physical Review B*, **2002**, 65,	3.3	329
646	Maximum noble-metal efficiency in catalytic materials: atomically dispersed surface platinum. *Angewandte Chemie - International Edition*, **2014**, 53, 10525-30	16.4	297
645	Ab Initio Cluster Model Calculations on the Chemisorption of CO2 and SO2 Probe Molecules on MgO and CaO (100) Surfaces. A Theoretical Measure of Oxide Basicity. *Journal of the American Chemical Society*, **1994**, 116, 10152-10158	16.4	274
644	Mechanisms responsible for chemical shifts of core-level binding energies and their relationship to chemical bonding. *Journal of Electron Spectroscopy and Related Phenomena*, **1999**, 100, 215-236	1.7	254
643	Magnetic coupling in biradicals, binuclear complexes and wide-gap insulators: a survey of ab initio wave function and density functional theory approaches. *Theoretical Chemistry Accounts*, **2000**, 104, 265-272	1.9	253
642	Antiferromagnetic Exchange Interactions from Hybrid Density Functional Theory. *Physical Review Letters*, **1997**, 79, 1539-1542	7.4	252
641	Decomposition of the chemisorption bond by constrained variations: Order of the variations and construction of the variational spaces. *Journal of Chemical Physics*, **1992**, 96, 8962-8970	3.9	196
640	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3832-9	6.4	187
639	A unified view of the theoretical description of magnetic coupling in molecular chemistry and solid state physics. *Physical Chemistry Chemical Physics*, **2006**, 8, 1645-59	3.6	184
638	Performance of the M06 family of exchange-correlation functionals for predicting magnetic coupling in organic and inorganic molecules. *Journal of Chemical Physics*, **2008**, 128, 114103	3.9	179
637	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. *Journal of Materials Chemistry*, **2010**, 20, 10535		168

636	CO2 hydrogenation on Au/TiC, Cu/TiC, and Ni/TiC catalysts: Production of CO, methanol, and methane. *Journal of Catalysis*, **2013**, 307, 162-169	7.3	162
635	A systematic density functional theory study of the electronic structure of bulk and (001) surface of transition-metals carbides. *Journal of Chemical Physics*, **2005**, 122, 174709	3.9	157
634	Establishing the Accuracy of Broadly Used Density Functionals in Describing Bulk Properties of Transition Metals. *Journal of Chemical Theory and Computation*, **2013**, 9, 1631-40	6.4	153
633	Atomic and electronic structure of molybdenum carbide phases: bulk and low Miller-index surfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 12617-25	3.6	151
632	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. *Chemical Communications*, **2010**, 46, 5936-8	5.8	145
631	Ab Initio Modeling of the Metal□Support Interface: The Interaction of Ni, Pd, and Pt on MgO(100). *Journal of Physical Chemistry B*, **1998**, 102, 1430-1436	3.4	145
630	First principles analysis of the stability and diffusion of oxygen vacancies in metal oxides. *Physical Review Letters*, **2004**, 93, 225502	7.4	144
629	Graphene on Ni(111): Coexistence of Different Surface Structures. *Journal of Physical Chemistry Letters*, **2011**, 2, 759-764	6.4	139
628	First-principles calculations of the atomic and electronic structure of F centers in the bulk and on the (001) surface of SrTiO3. *Physical Review B*, **2006**, 73,	3.3	138
627	On the activation of molecular hydrogen by gold: a theoretical approximation to the nature of potential active sites. *Chemical Communications*, **2007**, 3371-3	5.8	135
626	Adhesion energy of Cu atoms on the MgO(001) surface. *Journal of Chemical Physics*, **1999**, 110, 4873-4879	3.9	134
625	Active sites for H2 adsorption and activation in Au/TiO2 and the role of the support. *Journal of Physical Chemistry A*, **2009**, 113, 3750-7	2.8	133
624	Understanding the reactivity of metallic nanoparticles: beyond the extended surface model for catalysis. *Chemical Society Reviews*, **2014**, 43, 4922-39	58.5	132
623	The bending machine: CO2 activation and hydrogenation on □MoC(001) and □Mo2C(001) surfaces. *Physical Chemistry Chemical Physics*, **2014**, 16, 14912-21	3.6	131
622	Multiconfigurational Perturbation Theory: An Efficient Tool to Predict Magnetic Coupling Parameters in Biradicals, Molecular Complexes, and Ionic Insulators. *Journal of Physical Chemistry A*, **2001**, 105, 11371-11378	2.8	123
621	Bonding Mechanisms of Graphene on Metal Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 7360-7368	4.8	121
620	Magnetic coupling in ionic solids studied by density functional theory. *Journal of Chemical Physics*, **1998**, 108, 2519-2527	3.9	121
619	Accounting for van der Waals interactions between adsorbates and surfaces in density functional theory based calculations: selected examples. *RSC Advances*, **2013**, 3, 13085	3.7	120

618	Low-basicity oxygen atoms: a key in the search for propylene epoxidation catalysts. *Angewandte Chemie - International Edition*, **2007**, 46, 2055-8	16.4	117
617	Extent and limitations of density-functional theory in describing magnetic systems. *Physical Review B*, **2004**, 70,	3.3	116
616	Transition metal carbides as novel materials for CO2 capture, storage, and activation. *Energy and Environmental Science*, **2016**, 9, 141-144	35.4	115
615	Studies of the Cu?O bond in cupric oxide by X-ray photoelectron spectroscopy and ab initio electronic structure models. *Journal of Electron Spectroscopy and Related Phenomena*, **1992**, 59, 255-269	1.7	115
614	Density functional studies of model cerium oxide nanoparticles. *Physical Chemistry Chemical Physics* , **2008**, 10, 5730-8	3.6	114
613	Local character of magnetic coupling in ionic solids. *Physical Review B*, **1999**, 59, R6593-R6596	3.3	114
612	On the Promoting Role of Ag in Selective Hydrogenation Reactions over Pd□Ag Bimetallic Catalysts: A Theoretical Study. *Journal of Physical Chemistry C*, **2007**, 111, 6852-6856	3.8	113
611	Methane activation by platinum: critical role of edge and corner sites of metal nanoparticles. *Chemistry - A European Journal*, **2010**, 16, 6530-9	4.8	112
610	CO2 Activation and Methanol Synthesis on Novel Au/TiC and Cu/TiC Catalysts. *Journal of Physical Chemistry Letters*, **2012**, 3, 2275-80	6.4	111
609	Ultralow-density nanocage-based metal-oxide polymorphs. *Physical Review Letters*, **2007**, 99, 235502	7.4	111
608	Theoretical analysis of the bonding of oxygen to Cu(100). *Physical Review B*, **1990**, 42, 10852-10857	3.3	110
607	Electronic structure of a neutral oxygen vacancy in SrTiO3. *Physical Review B*, **2003**, 68,	3.3	108
606	Accurate prediction of large antiferromagnetic interactions in high- T(c) HgBa2Ca(n-1)Cu(n)O(2n+2+delta) (n = 2,3) superconductor parent compounds. *Physical Review Letters*, **2000**, 84, 1579-82	7.4	107
605	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	3.8	106
604	Why copper is intrinsically more selective than silver in alkene epoxidation: ethylene oxidation on Cu(111) versus Ag(111). *Journal of the American Chemical Society*, **2005**, 127, 10774-5	16.4	105
603	Transition metal adatoms on graphene: A systematic density functional study. *Carbon*, **2015**, 95, 525-534	10.4	103
602	Density Functional Theory Study of the Interaction of Cu, Ag, and Au Atoms with the Regular CeO2 (111) Surface. *Journal of Physical Chemistry C*, **2010**, 114, 1934-1941	3.8	103
601	Critical size for O(2) dissociation by au nanoparticles. *ChemPhysChem*, **2009**, 10, 348-51	3.2	102

600	Restricted Ensemble-Referenced Kohn-Sham versus Broken Symmetry Approaches in Density Functional Theory: Magnetic Coupling in Cu Binuclear Complexes. *Journal of Chemical Theory and Computation*, **2007**, 3, 764-74	6.4	102
599	Mechanism of selective alcohol oxidation to aldehydes on gold catalysts: Influence of surface roughness on reactivity. *Journal of Catalysis*, **2011**, 278, 50-58	7.3	101
598	Measures of ionicity of alkaline-earth oxides from the analysis of ab initio cluster wave functions. *Physical Review B*, **1993**, 48, 11573-11582	3.3	101
597	Ab Initio Study of the Exchange Coupling in Oxalato-Bridged Cu(II) Dinuclear Complexes. *Journal of Physical Chemistry A*, **2000**, 104, 9983-9989	2.8	100
596	When the reporter induces the effect: unusual IR spectra of CO on Au1/MgO(001)/Mo(001). *Angewandte Chemie - International Edition*, **2006**, 45, 2633-5	16.4	98
595	Comparative study of the molecular electrostatic potential obtained from different wavefunctions. Reliability of the semiempirical MNDO wavefunction. *Journal of Computational Chemistry*, **1990**, 11, 416-430	3.5	97
594	Ab initio theoretical comparative study of magnetic coupling in KNiF3sand K2 NiF4s. *Physical Review B*, **1997**, 55, 4129-4137	3.3	96
593	Comment on "about the calculation of exchange coupling constants using density-functional theory: the role of the self-interaction error" [J. Chem. Phys. 123, 164110 (2005)]. *Journal of Chemical Physics*, **2006**, 124, 107101; author reply 107102	3.9	95
592	CO2 abatement using two-dimensional MXene carbides. *Journal of Materials Chemistry A*, **2018**, 6, 3381-3385	13	93
591	Highly Active Au/δ-MoC and Cu/δ-MoC Catalysts for the Conversion of CO2: The Metal/C Ratio as a Key Factor Defining Activity, Selectivity, and Stability. *Journal of the American Chemical Society*, **2016**, 138, 8269-78	16.4	92
590	Approaching nanoscale oxides: models and theoretical methods. *Chemical Society Reviews*, **2009**, 38, 2657-70	58.5	92
589	Understanding Ceria Nanoparticles from First-Principles Calculations. *Journal of Physical Chemistry C*, **2007**, 111, 10142-10145	3.8	92
588	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. *Physical Chemistry Chemical Physics*, **2004**, 6, 314-318	3.6	92
587	Formation of Superoxide Anions on Ceria Nanoparticles by Interaction of Molecular Oxygen with Ce3+ Sites. *Journal of Physical Chemistry C*, **2011**, 115, 5817-5822	3.8	90
586	Influence of step sites in the molecular mechanism of the water gas shift reaction catalyzed by copper. *Journal of Catalysis*, **2009**, 268, 131-141	7.3	88
585	MXenes: New Horizons in Catalysis. *ACS Catalysis*, **2020**, 10, 13487-13503	13.1	87
584	On modelling the interaction of CO on the MgO(100) surface. *Surface Science*, **1995**, 327, 59-73	1.8	87
583	A systematic study of the structure and bonding of halogens on low-index transition metal surfaces. *Journal of Physical Chemistry B*, **2006**, 110, 11894-906	3.4	85

582	Adsorption of Cu, Pd, and Cs Atoms on Regular and Defect Sites of the SiO2 Surface. *Journal of the American Chemical Society*, **1999**, 121, 813-821	16.4	81
581	Role of Au-C interactions on the catalytic activity of au nanoparticles supported on TiC(001) toward molecular oxygen dissociation. *Journal of the American Chemical Society*, **2010**, 132, 3177-86	16.4	79
580	Effect of the exchange-correlation potential and of surface relaxation on the description of the H(2)O dissociation on Cu(111). *Journal of Chemical Physics*, **2009**, 130, 224702	3.9	79
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577	Nature of Ag Islands and Nanoparticles on the CeO2(111) Surface. *Journal of Physical Chemistry C*, **2012**, 116, 1122-1132	3.8	77
576	Good performance of the M06 family of hybrid meta generalized gradient approximation density functionals on a difficult case: CO adsorption on MgO(001). *Journal of Chemical Physics*, **2008**, 129, 124710	3.9	76
575	Ab Initio Cluster Model Study of the Chemisorption of CO on Low-Index Platinum Surfaces. *Journal of Physical Chemistry B*, **1999**, 103, 5246-5255	3.4	76
574	Bandgap engineering of graphene by physisorbed adsorbates. *Advanced Materials*, **2011**, 23, 2638-43	24	75
573	The conversion of CO2 to methanol on orthorhombic □Mo2C and Cu/□Mo2C catalysts: mechanism for admetal induced change in the selectivity and activity. *Catalysis Science and Technology*, **2016**, 6, 6766-6777	5.5	74
572	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. *Journal of Catalysis*, **2010**, 276, 92-100	7.3	74
571	Importance of Madelung potential in quantum chemical modeling of ionic surfaces. *Journal of Computational Chemistry*, **1997**, 18, 617-628	3.5	74
570	Theoretical study of bulk and surface oxygen and aluminum vacancies in □Al2O3. *Physical Review B*, **2004**, 69,	3.3	74
569	Reliability of range-separated hybrid functionals for describing magnetic coupling in molecular systems. *Journal of Chemical Physics*, **2008**, 129, 184110	3.9	73
568	When Langmuir is too simple: H2 dissociation on Pd(111) at high coverage. *Physical Review Letters*, **2004**, 93, 146103	7.4	73
567	Madelung fields from optimized point charges for ab initio cluster model calculations on ionic systems. *Journal of Computational Chemistry*, **1993**, 14, 680-684	3.5	73
566	Reactivity of Transition Metals (Pd, Pt, Cu, Ag, Au) toward Molecular Hydrogen Dissociation: Extended Surfaces versus Particles Supported on TiC(001) or Small Is Not Always Better and Large Is Not Always Bad. *Journal of Physical Chemistry C*, **2011**, 115, 11666-11672	3.8	72
565	Rigorous characterization of oxygen vacancies in ionic oxides. *Physical Review B*, **2002**, 66,	3.3	72

564	Theoretical Confirmation of the Enhanced Facility to Increase Oxygen Vacancy Concentration in TiO2 by Iron Doping. *Journal of Physical Chemistry C*, **2010**, 114, 6511-6517	3.8	71
563	Spin Symmetry Requirements in Density Functional Theory: The Proper Way to Predict Magnetic Coupling Constants in Molecules and Solids. *Theoretical Chemistry Accounts*, **2006**, 116, 587-597	1.9	71
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561	Theoretical approaches to excited-state-related phenomena in oxide surfaces. *Chemical Reviews*, **2013**, 113, 4456-95	68.1	69
560	Effects of deposited Pt particles on the reducibility of CeO2(111). *Physical Chemistry Chemical Physics*, **2011**, 13, 11384-92	3.6	69
559	Electronic and magnetic structure of bulk cobalt: the alpha, beta, and epsilon-phases from density functional theory calculations. *Journal of Chemical Physics*, **2010**, 133, 024701	3.9	69
558	Towards an ab initio description of magnetism in ionic solids. *Physical Review Letters*, **1993**, 71, 3549-3552	7.4	69
557	Effective and Highly Selective CO Generation from CO2 Using a Polycrystalline Mo2C Catalyst. *ACS Catalysis*, **2017**, 7, 4323-4335	13.1	68
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551	Adsorption, Oxidation State, and Diffusion of Pt Atoms on the CeO2(111) Surface. *Journal of Physical Chemistry C*, **2010**, 114, 14202-14207	3.8	64
550	Edge sites as a gate for subsurface carbon in palladium nanoparticles. *Journal of Catalysis*, **2009**, 266, 59-63	7.3	64
549	Desulfurization of thiophene on Au/TiC(001): Au-C interactions and charge polarization. *Journal of the American Chemical Society*, **2009**, 131, 8595-602	16.4	64
548	Dissociation of SO2 on Au/TiC(001): effects of Au-C interactions and charge polarization. *Angewandte Chemie - International Edition*, **2008**, 47, 6685-9	16.4	64
547	Evidence for spontaneous CO2 activation on cobalt surfaces. *Chemical Physics Letters*, **2008**, 454, 262-268	2.5	64

546	Chemisorption of atomic chlorine on metal surfaces and the interpretation of the induced work function changes. *Surface Science*, **2005**, 574, 297-305	1.8	64
545	Theoretical aspects of heterogeneous catalysis: Applications of density functional methods. *Catalysis Today*, **2005**, 105, 2-16	5.3	63
544	Ab initio study of the optical transitions of F centers at low-coordinated sites of the MgO surface. *Surface Science*, **1999**, 429, 217-228	1.8	63
543	Quantum-Chemical Study of Electrochemical Promotion in Catalysis. *The Journal of Physical Chemistry*, **1996**, 100, 16653-16661		63
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537	Validation of Koopmans' theorem for density functional theory binding energies. *Physical Chemistry Chemical Physics*, **2015**, 17, 4015-9	3.6	60
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535	Adsorption of gold on TiC(001): Au-C interactions and charge polarization. *Journal of Chemical Physics*, **2007**, 127, 211102	3.9	59
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531	On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO2(111). *Journal of Chemical Physics*, **2009**, 131, 094702	3.9	58
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