Josep Manel Ricart

List of Publications by Year
in descending order

82	3,377	136950 32	149698 56
papers	citations	h-index	g-index

83	83	83	3629
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nâ•N Bond Cleavage by Tantalum Hydride Complexes: Mechanistic Insights and Reactivity. Inorganic Chemistry, 2022, 61, 474-485.	4.0	5
2	Peptide Hydrolysis by Metal (Oxa)cyclen Complexes: Revisiting the Mechanism and Assessing Ligand Effects. Inorganic Chemistry, 2021, 60, 807-815.	4.0	5
3	Regioselectivity Control in Pd-Catalyzed Telomerization of Isoprene Enabled by Solvent and Ligand Selection. ACS Catalysis, 2020, 10, 11458-11465.	11.2	9
4	A Bridging bis-Allyl Titanium Complex: Mechanistic Insights into the Electronic Structure and Reactivity. Inorganic Chemistry, 2019, 58, 12157-12166.	4.0	4
5	Understanding the mechanism of transition metal-free anti addition to alkynes: the selenoboration case. Catalysis Science and Technology, 2018, 8, 3617-3628.	4.1	13
6	Understanding the Regioselectivity of Aromatic Hydroxylation over Divanadium-Substituted Î³-Keggin Polyoxotungstate. ACS Catalysis, 2017, 7, 8514-8523.	11.2	23
7	Exploring the activity of a novel Au/TiC(001) model catalyst towards CO and CO2 hydrogenation. Surface Science, 2015, 640, 141-149.	1.9	17
8	Charge Polarization at a Auâ€“TiC Interface and the Generation of Highly Active and Selective Catalysts for the Lowâ€Temperature Waterâ€“Gas Shift Reaction. Angewandte Chemie - International Edition, 2014, 53, 11270-11274.	13.8	67
9	New Insights into the Structure of the C-Terminated Î²-Mo₂C (001) Surface from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 19224-19231.	3.1	13
10	When reconstruction comes around: Ni, Cu, and Au adatoms on Î'-MoC(001). Surface Science, 2014, 624, 32-36.	1.9	5
11	Theoretical and experimental study of the interaction of CO on TiC surfaces: Regular versus low coordinated sites. Surface Science, 2013, 613, 63-73.	1.9	5
12	Theoretical Study of the Interaction of CO on TiC(001) and Au Nanoparticles Supported on TiC(001): Probing the Nature of the Au/TiC Interface. Journal of Physical Chemistry C, 2011, 115, 22495-22504.	3.1	17
13	Origin of the size dependence of Au nanoparticles toward molecular oxygen dissociation. Theoretical Chemistry Accounts, 2011, 128, 675-681.	1.4	32
14	Theoretical Simulation of Temperature Programmed Desorption of Molecular Oxygen on Isolated Au Nanoparticles from Density Functional Calculations and Microkinetics Models. Journal of Physical Chemistry C, 2010, 114, 5101-5106.	3.1	13
15	O₂ Activation by Au₅ Clusters Stabilized on Clean and Electron-Rich MgO Stepped Surfaces. Journal of Physical Chemistry C, 2010, 114, 16973-16978.	3.1	33
16	O2 adsorption and dissociation on neutral, positively and negatively charged Aun (n = 5â€“79) clusters. Physical Chemistry Chemical Physics, 2010, 12, 10723.	2.8	50
17	Mechanism of ammonia oxidation over PGM (Pt, Pd, Rh) wires by temporal analysis of products and density functional theory. Journal of Catalysis, 2009, 261, 217-223.	6.2	47
18	Critical Size for O₂ Dissociation by Au Nanoparticles. ChemPhysChem, 2009, 10, 348-351.	2.1	108

#	Article	IF	Citations
19	Influence of the exchangeâ€“correlation potential on the description of the molecular mechanism of oxygen dissociation by Au nanoparticles. Theoretical Chemistry Accounts, 2009, 123, 119-126.	1.4	47
20	On the effectiveness of partial oxidation of propylene by gold: A density functional theory study. Journal of Molecular Catalysis A, 2009, 306, 6-10.	4.8	31
21	Growth and properties of Au nanowires. Molecular Simulation, 2009, 35, 1051-1056.	2.0	4
22	Density functional studies of coinage metal nanoparticles: scalability of their properties to bulk. Theoretical Chemistry Accounts, 2008, 120, 565-573.	1.4	61
23	The chemistry of chlorine on Ag(1 1 1) over the sub-monolayer range: A density functional theory investigation. Surface Science, 2008, 602, 2639-2642.	1.9	9
24	Pt(100)-Catalyzed Ammonia Oxidation Studied by DFT: Mechanism and Microkinetics. Journal of Physical Chemistry C, 2008, 112, 13554-13562.	3.1	107
25	Adsorption properties and vibrational spectra of propyne adsorbed on Rh(111). Comparison with other (111) metal surfaces. Physical Chemistry Chemical Physics, 2007, 9, 311-317.	2.8	5
26	Ammonia Dissociation on Pt{100}, Pt{111}, and Pt{211}:â€‰ A Comparative Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 17551-17557.	3.1	72
27	Ammonia Dehydrogenation over Platinum-Group Metal Surfaces. Structure, Stability, and Reactivity of Adsorbed NHxSpecies. Journal of Physical Chemistry C, 2007, 111, 860-868.	3.1	118
28	Theoretical study of dehydrogenation and isomerisation reactions of propylene on Pt(111). Journal of Catalysis, 2006, 241, 115-122.	6.2	43
29	Acetylene Decomposition on Rh(100): Theory and Experiment. ChemPhysChem, 2006, 7, 1068-1074.	2.1	6
30	Comparative theoretical study of the structure and bonding of propyne on the Pt(111) and Pd(111) surfaces. Chemical Physics, 2005, 309, 33-39.	1.9	15
31	Structure and catalytic processes of N-containing species on Rh(111) from first principles. Journal of Catalysis, 2005, 232, 179-185.	6.2	33
32	Selectivity Control for the Catalytic 1,3-Butadiene Hydrogenation on Pt(111) and Pd(111) Surfaces:Â Radical versus Closed-Shell Intermediates. Journal of Physical Chemistry B, 2005, 109, 14175-14182.	2.6	51
33	Competitive CN and N2 formation on Rh(1 1 1): a case of entropic stabilization. Chemical Physics Letters, 2004, 385, 52-54.	2.6	16
34	Structure and bonding mechanism of cyanide adsorbed on Pt(111). Surface Science, 2004, 558, 111-121.	1.9	34
35	Comparative DFT study of the adsorption of 1,3-butadiene, 1-butene and 2-cis/trans-butenes on the Pt(111) and Pd(111) surfaces. Surface Science, 2004, 549, 121-133.	1.9	90
36	Theoretical study of propene adsorbed on sulphated Pt(111). Chemical Physics Letters, 2004, 399, 295-299.	2.6	4

#	Article	IF	Citations
37	Structural and Spectroelectrochemical Study of Carbonate and Bicarbonate Adsorbed on Pt(111) and Pd/Pt(111) Electrodes. Journal of Physical Chemistry B, 2004, 108, 17928-17939.	2.6	39
38	Theoretical Studies of N2O Adsorption and Reactivity to N2and NO on Rh(111). Journal of Physical Chemistry B, 2004, 108, 17921-17927.	2.6	38
39	Theoretical Interpretation of the IR Spectrum of Propyne on Cu(111). Journal of Physical Chemistry B, 2004, 108, 18297-18305.	2.6	21
40	Site preference of CO chemisorbed on Pt(111) from density functional calculations. Surface Science, 2003, 530, 71-87.	1.9	155
41	Structure and bonding of propyne on Cu(111) from density functional periodic and cluster models. Journal of Chemical Physics, 2002, 116, 1165-1170.	3.0	20
42	A density functional study of the adsorption of CO on Rh(111). Physical Chemistry Chemical Physics, 2002, 4, 5372-5376.	2.8	10
43	Adsorption of CO and CNâ˜' on transition metal surfaces: a comparative study of the bonding mechanism. Surface Science, 2002, 497, 139-154.	1.9	36
44	Theoretical study of the structure of propene adsorbed on Pt(). Surface Science, 2002, 519, 250-258.	1.9	31
45	Assignment of the vibrational features in the Rh(111)â€“(2Ã—2)-3CO adsorption structure using density functional theory calculations. Chemical Physics Letters, 2002, 354, 503-507.	2.6	17
46	Adsorption of CO at Palladium Monolayers Deposited on Pt(111) Electrodes. Combined Spectroelectrochemical and Theoretical Study. Journal of Physical Chemistry B, 2001, 105, 7263-7271.	2.6	39
47	A theoretical investigation of the binding of TiCln to MgCl2. Surface Science, 2001, 490, 237-250.	1.9	35
48	Chemisorption of molecular oxygen on Cu(1 0 0): a Hartreeâ€“Fock and density functional study. Journal of Molecular Catalysis A, 2001, 167, 109-113.	4.8	11
49	Density functional studies on the adsorption and decomposition of SO2 on Cu(100). Journal of Chemical Physics, 2001, 115, 454-465.	3.0	51
50	Adsorption of carbon monoxide on Pt{100} surfaces: dependence of the CO stretching vibrational frequency on surface coverage. Surface Science, 2000, 460, 101-111.	1.9	30
51	Theoretical study of CO2 activation on Pt(111) induced by coadsorbed K atoms. Surface Science, 2000, 460, 170-181.	1.9	39
52	A Theoretical Study of Catalytic Coupling of Propyne on Cu{111}. Journal of the American Chemical Society, 2000, 122, 7573-7578.	13.7	27
53	Ab initio cluster model comparative study of atomic oxygen and sulfur chemisorption on Pt(111) surface: relevance to heterogeneous catalysis. Catalysis Today, 1999, 50, 613-620.	4.4	7
54	Ab initio cluster model study of electric field effects for terminal and bridge bonded CO on Pt(100). Electrochimica Acta, 1999, 45, 639-644.	5.2	23

#	Article	IF	Citations
55	Ab Initio Cluster Model Study of the Chemisorption of CO on Low-Index Platinum Surfaces. Journal of Physical Chemistry B, 1999, 103, 5246-5255.	2.6	78
56	Electric field effects on the vibrational frequency and bonding mechanism of CO on Pt(111). Electrochimica Acta, 1998, 44, 1213-1220.	5.2	47
57	Bonding of vinylidene on Pd(111). Computational and Theoretical Chemistry, 1998, 458, 123-129.	1.5	12
58	Density functional study of atomic nitrogen and oxygen chemisorption on model clusters simulating the Cu and Ag (100) surfaces. Journal of Molecular Catalysis A, 1997, 119, 387-392.	4.8	9
59	Charge displacement analysis: A new general method to estimate atomic charges in molecules and clusters. Journal of Molecular Catalysis A, 1997, 119, 3-10.	4.8	20
60	The interpretation of X-ray photoelectron spectra of pyrolized S-containing carbonaceous materials. Fuel, 1997, 76, 1347-1352.	6.4	8
61	Physical mechanisms responsible for core-level shifts of alkali metals adsorbed on Si(111). Surface Science, 1996, 364, 89-98.	1.9	16
62	Computational study of the conformational profiles of model bis-cystine cyclic peptides. International Journal of Biological Macromolecules, 1996, 18, 263-274.	7.5	0
63	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.	13.7	490
64	Consequences of chemical bonding on the adiabaticity of gas-surface reactions. Computational and Theoretical Chemistry, 1996, 371, 257-267.	1.5	4
65	The importance of correlation effects on the bonding of atomic oxygen on Pt(111). Journal of Chemical Physics, 1996, 105, 7192-7199.	3.0	22
66	Theoretical evidence for the existence of excitons in MgO. Chemical Physics Letters, 1995, 239, 263-266.	2.6	13
67	Performance of correlation functionals inab initiochemisorption cluster-model calculations: Alkali metals on Si(111). Physical Review B, 1995, 52, 11998-12005.	3.2	6
68	Electronic and magnetic structure ofKNiF3perovskite. Physical Review B, 1995, 52, 2381-2389.	3.2	79
69	Nature of bonding of alkali metals to Si(111). Physical Review B, 1995, 51, 1581-1592.	3.2	30
70	Superexchange interaction in K2NiF4: an ab initio Hartree-Fock study. Journal of Physics Condensed Matter, 1995, 7, 7997-8007.	1.8	26
71	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.	13.7	301
72	A theoretical study of the adsorption and reaction of SO2 at surface and step sites of the MgO(100) surface. Surface Science, 1994, 315, 337-350.	1.9	99

#	Article	IF	Citations
73	Evidence for two different bonding mechanisms of Al on Si(111). Physical Review B, 1993, 47, 2417-2419.	3.2	11
74	Chemisorption of group-III metals on the Si(111) and Ge(111) surfaces: Anab initiostudy. Physical Review B, 1990, 42, 5212-5220.	3.2	28
75	Electronic structure of Rh, RhH, and Rh2 as derived from ab initio (configuration interaction) calculations. Journal of Chemical Physics, 1990, 93, 2603-2610.	3.0	35
76	Ab initio selfâ€consistent field and configuration interaction study of Cu5O and Ag5O as models for oxygen chemisorption on Cu(100) and Ag(100). Journal of Chemical Physics, 1989, 91, 5466-5475.	3.0	32
77	Molecular structure and vibrational frequencies of AlxOy (x=1,2; yâ©½3) derived from ab initio calculations. Chemical Physics Letters, 1988, 144, 373-377.	2.6	50
78	Chemisorption of atomic aluminum on Si(111): Evidence for an adsorbate-induced relaxation based onab initiocluster-model calculations. Physical Review B, 1988, 38, 10700-10710.	3.2	21
79	Theoretical evidence for two geometrical isomers of silver oxide (AgO2). Journal of the American Chemical Society, 1986, 108, 7893-7897.	13.7	15
80	The effect of electron correlation in the interaction of atomic hydrogen with Ben clusters 3â‰nâ‰7. Journal of Chemical Physics, 1986, 84, 3311-3316.	3.0	17
81	Ab initiocluster-model study of the on-top chemisorption of F and Cl on Si(111) and Ge(111) surfaces. Physical Review B, 1985, 31, 8068-8075.	3.2	49
82	Conformational basis of N-glycosylation of proteins: conformational analysis of Ac-Asn-Ala-Thr-NH2. International Journal of Biological Macromolecules, 1983, 5, 279-282.	7.5	4