

Josep Manel Ricart

List of Publications by Year in descending order

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82
papers

3,377
citations

136950

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83
docs citations

83
times ranked

3629
citing authors

#	ARTICLE	IF	CITATIONS
1	Origin of the Large N 1s Binding Energy in X-ray Photoelectron Spectra of Calcined Carbonaceous Materials. <i>Journal of the American Chemical Society</i> , 1996, 118, 8071-8076.	13.7	490
2	Ab Initio Cluster Model Calculations on the Chemisorption of CO ₂ and SO ₂ Probe Molecules on MgO and CaO (100) Surfaces. A Theoretical Measure of Oxide Basicity. <i>Journal of the American Chemical Society</i> , 1994, 116, 10152-10158.	13.7	301
3	Site preference of CO chemisorbed on Pt(111) from density functional calculations. <i>Surface Science</i> , 2003, 530, 71-87.	1.9	155
4	Ammonia Dehydrogenation over Platinum-Group Metal Surfaces. Structure, Stability, and Reactivity of Adsorbed NH _x Species. <i>Journal of Physical Chemistry C</i> , 2007, 111, 860-868.	3.1	118
5	Critical Size for O ₂ Dissociation by Au Nanoparticles. <i>ChemPhysChem</i> , 2009, 10, 348-351.	2.1	108
6	Pt(100)-Catalyzed Ammonia Oxidation Studied by DFT: Mechanism and Microkinetics. <i>Journal of Physical Chemistry C</i> , 2008, 112, 13554-13562.	3.1	107
7	A theoretical study of the adsorption and reaction of SO ₂ at surface and step sites of the MgO(100) surface. <i>Surface Science</i> , 1994, 315, 337-350.	1.9	99
8	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. <i>Surface Science</i> , 2004, 549, 121-133.	1.9	90
9	Electronic and magnetic structure of KNiF ₃ perovskite. <i>Physical Review B</i> , 1995, 52, 2381-2389.	3.2	79
10	Ab Initio Cluster Model Study of the Chemisorption of CO on Low-Index Platinum Surfaces. <i>Journal of Physical Chemistry B</i> , 1999, 103, 5246-5255.	2.6	78
11	Ammonia Dissociation on Pt{100}, Pt{111}, and Pt{211}: A Comparative Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 17551-17557.	3.1	72
12	Charge Polarization at a Au/TiC Interface and the Generation of Highly Active and Selective Catalysts for the Low-Temperature Water-Gas Shift Reaction. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11270-11274.	13.8	67
13	Density functional studies of coinage metal nanoparticles: scalability of their properties to bulk. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 565-573.	1.4	61
14	Density functional studies on the adsorption and decomposition of SO ₂ on Cu(100). <i>Journal of Chemical Physics</i> , 2001, 115, 454-465.	3.0	51
15	Selectivity Control for the Catalytic 1,3-Butadiene Hydrogenation on Pt(111) and Pd(111) Surfaces: A Radical versus Closed-Shell Intermediates. <i>Journal of Physical Chemistry B</i> , 2005, 109, 14175-14182.	2.6	51
16	Molecular structure and vibrational frequencies of Al _x O _y (x=1,2; y=1/2,3) derived from ab initio calculations. <i>Chemical Physics Letters</i> , 1988, 144, 373-377.	2.6	50
17	O ₂ adsorption and dissociation on neutral, positively and negatively charged Au _n (n = 5-79) clusters. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10723.	2.8	50
18	Ab initio cluster-model study of the on-top chemisorption of F and Cl on Si(111) and Ge(111) surfaces. <i>Physical Review B</i> , 1985, 31, 8068-8075.	3.2	49

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19	Electric field effects on the vibrational frequency and bonding mechanism of CO on Pt(111). <i>Electrochimica Acta</i> , 1998, 44, 1213-1220.	5.2	47
20	Mechanism of ammonia oxidation over PGM (Pt, Pd, Rh) wires by temporal analysis of products and density functional theory. <i>Journal of Catalysis</i> , 2009, 261, 217-223.	6.2	47
21	Influence of the exchangeâ€‘correlation potential on the description of the molecular mechanism of oxygen dissociation by Au nanoparticles. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 119-126.	1.4	47
22	Theoretical study of dehydrogenation and isomerisation reactions of propylene on Pt(111). <i>Journal of Catalysis</i> , 2006, 241, 115-122.	6.2	43
23	Theoretical study of CO ₂ activation on Pt(111) induced by coadsorbed K atoms. <i>Surface Science</i> , 2000, 460, 170-181.	1.9	39
24	Adsorption of CO at Palladium Monolayers Deposited on Pt(111) Electrodes. Combined Spectroelectrochemical and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7263-7271.	2.6	39
25	Structural and Spectroelectrochemical Study of Carbonate and Bicarbonate Adsorbed on Pt(111) and Pd/Pt(111) Electrodes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17928-17939.	2.6	39
26	Theoretical Studies of N ₂ O Adsorption and Reactivity to N ₂ and NO on Rh(111). <i>Journal of Physical Chemistry B</i> , 2004, 108, 17921-17927.	2.6	38
27	Adsorption of CO and CNâˆ’ on transition metal surfaces: a comparative study of the bonding mechanism. <i>Surface Science</i> , 2002, 497, 139-154.	1.9	36
28	Electronic structure of Rh, RhH, and Rh ₂ as derived from ab initio (configuration interaction) calculations. <i>Journal of Chemical Physics</i> , 1990, 93, 2603-2610.	3.0	35
29	A theoretical investigation of the binding of TiCl _n to MgCl ₂ . <i>Surface Science</i> , 2001, 490, 237-250.	1.9	35
30	Structure and bonding mechanism of cyanide adsorbed on Pt(111). <i>Surface Science</i> , 2004, 558, 111-121.	1.9	34
31	Structure and catalytic processes of N-containing species on Rh(111) from first principles. <i>Journal of Catalysis</i> , 2005, 232, 179-185.	6.2	33
32	O ₂ Activation by Au ₅ Clusters Stabilized on Clean and Electron-Rich MgO Stepped Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16973-16978.	3.1	33
33	Ab initio self-consistent field and configuration interaction study of Cu ₅ O and Ag ₅ O as models for oxygen chemisorption on Cu(100) and Ag(100). <i>Journal of Chemical Physics</i> , 1989, 91, 5466-5475.	3.0	32
34	Origin of the size dependence of Au nanoparticles toward molecular oxygen dissociation. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 675-681.	1.4	32
35	Theoretical study of the structure of propene adsorbed on Pt(). <i>Surface Science</i> , 2002, 519, 250-258.	1.9	31
36	On the effectiveness of partial oxidation of propylene by gold: A density functional theory study. <i>Journal of Molecular Catalysis A</i> , 2009, 306, 6-10.	4.8	31

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37	Nature of bonding of alkali metals to Si(111). <i>Physical Review B</i> , 1995, 51, 1581-1592.	3.2	30
38	Adsorption of carbon monoxide on Pt{100} surfaces: dependence of the CO stretching vibrational frequency on surface coverage. <i>Surface Science</i> , 2000, 460, 101-111.	1.9	30
39	Chemisorption of group-III metals on the Si(111) and Ge(111) surfaces: An ab initio study. <i>Physical Review B</i> , 1990, 42, 5212-5220.	3.2	28
40	A Theoretical Study of Catalytic Coupling of Propyne on Cu{111}. <i>Journal of the American Chemical Society</i> , 2000, 122, 7573-7578.	13.7	27
41	Superexchange interaction in K ₂ NiF ₄ : an ab initio Hartree-Fock study. <i>Journal of Physics Condensed Matter</i> , 1995, 7, 7997-8007.	1.8	26
42	Ab initio cluster model study of electric field effects for terminal and bridge bonded CO on Pt(100). <i>Electrochimica Acta</i> , 1999, 45, 639-644.	5.2	23
43	Understanding the Regioselectivity of Aromatic Hydroxylation over Divanadium-Substituted \hat{I}^3 -Keggin Polyoxotungstate. <i>ACS Catalysis</i> , 2017, 7, 8514-8523.	11.2	23
44	The importance of correlation effects on the bonding of atomic oxygen on Pt(111). <i>Journal of Chemical Physics</i> , 1996, 105, 7192-7199.	3.0	22
45	Chemisorption of atomic aluminum on Si(111): Evidence for an adsorbate-induced relaxation based on ab initio cluster-model calculations. <i>Physical Review B</i> , 1988, 38, 10700-10710.	3.2	21
46	Theoretical Interpretation of the IR Spectrum of Propyne on Cu(111). <i>Journal of Physical Chemistry B</i> , 2004, 108, 18297-18305.	2.6	21
47	Charge displacement analysis: A new general method to estimate atomic charges in molecules and clusters. <i>Journal of Molecular Catalysis A</i> , 1997, 119, 3-10.	4.8	20
48	Structure and bonding of propyne on Cu(111) from density functional periodic and cluster models. <i>Journal of Chemical Physics</i> , 2002, 116, 1165-1170.	3.0	20
49	The effect of electron correlation in the interaction of atomic hydrogen with Ben clusters. <i>Journal of Chemical Physics</i> , 1986, 84, 3311-3316.	3.0	17
50	Assignment of the vibrational features in the Rh(111)-(2x2)-3CO adsorption structure using density functional theory calculations. <i>Chemical Physics Letters</i> , 2002, 354, 503-507.	2.6	17
51	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. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22495-22504.	3.1	17
52	Exploring the activity of a novel Au/TiC(001) model catalyst towards CO and CO ₂ hydrogenation. <i>Surface Science</i> , 2015, 640, 141-149.	1.9	17
53	Physical mechanisms responsible for core-level shifts of alkali metals adsorbed on Si(111). <i>Surface Science</i> , 1996, 364, 89-98.	1.9	16
54	Competitive CN and N ₂ formation on Rh(1 1 1): a case of entropic stabilization. <i>Chemical Physics Letters</i> , 2004, 385, 52-54.	2.6	16

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55	Theoretical evidence for two geometrical isomers of silver oxide (Ag ₂ O). Journal of the American Chemical Society, 1986, 108, 7893-7897.	13.7	15
56	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
57	Theoretical evidence for the existence of excitons in MgO. Chemical Physics Letters, 1995, 239, 263-266.	2.6	13
58	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
59	New Insights into the Structure of the C-Terminated \hat{I}^2 -Mo ₂ C (001) Surface from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 19224-19231.	3.1	13
60	Understanding the mechanism of transition metal-free <i>anti</i> addition to alkynes: the selenoboration case. Catalysis Science and Technology, 2018, 8, 3617-3628.	4.1	13
61	Bonding of vinylidene on Pd(111). Computational and Theoretical Chemistry, 1998, 458, 123-129.	1.5	12
62	Evidence for two different bonding mechanisms of Al on Si(111). Physical Review B, 1993, 47, 2417-2419.	3.2	11
63	Chemisorption of molecular oxygen on Cu(1 0 0): a Hartree-Fock and density functional study. Journal of Molecular Catalysis A, 2001, 167, 109-113.	4.8	11
64	A density functional study of the adsorption of CO on Rh(111). Physical Chemistry Chemical Physics, 2002, 4, 5372-5376.	2.8	10
65	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
66	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
67	Regioselectivity Control in Pd-Catalyzed Telomerization of Isoprene Enabled by Solvent and Ligand Selection. ACS Catalysis, 2020, 10, 11458-11465.	11.2	9
68	The interpretation of X-ray photoelectron spectra of pyrolyzed S-containing carbonaceous materials. Fuel, 1997, 76, 1347-1352.	6.4	8
69	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
70	Performance of correlation functionals in ab initio chemisorption cluster-model calculations: Alkali metals on Si(111). Physical Review B, 1995, 52, 11998-12005.	3.2	6
71	Acetylene Decomposition on Rh(100): Theory and Experiment. ChemPhysChem, 2006, 7, 1068-1074.	2.1	6
72	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

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73	Theoretical and experimental study of the interaction of CO on TiC surfaces: Regular versus low coordinated sites. <i>Surface Science</i> , 2013, 613, 63-73.	1.9	5
74	When reconstruction comes around: Ni, Cu, and Au adatoms on $\sqrt{3}\times\sqrt{3}$ -MoC(001). <i>Surface Science</i> , 2014, 624, 32-36.	1.9	5
75	Peptide Hydrolysis by Metal (Oxa)cyclen Complexes: Revisiting the Mechanism and Assessing Ligand Effects. <i>Inorganic Chemistry</i> , 2021, 60, 807-815.	4.0	5
76	N α -N Bond Cleavage by Tantalum Hydride Complexes: Mechanistic Insights and Reactivity. <i>Inorganic Chemistry</i> , 2022, 61, 474-485.	4.0	5
77	Conformational basis of N-glycosylation of proteins: conformational analysis of Ac-Asn-Ala-Thr-NH ₂ . <i>International Journal of Biological Macromolecules</i> , 1983, 5, 279-282.	7.5	4
78	Consequences of chemical bonding on the adiabaticity of gas-surface reactions. <i>Computational and Theoretical Chemistry</i> , 1996, 371, 257-267.	1.5	4
79	Theoretical study of propene adsorbed on sulphated Pt(111). <i>Chemical Physics Letters</i> , 2004, 399, 295-299.	2.6	4
80	Growth and properties of Au nanowires. <i>Molecular Simulation</i> , 2009, 35, 1051-1056.	2.0	4
81	A Bridging bis-Allyl Titanium Complex: Mechanistic Insights into the Electronic Structure and Reactivity. <i>Inorganic Chemistry</i> , 2019, 58, 12157-12166.	4.0	4
82	Computational study of the conformational profiles of model bis-cystine cyclic peptides. <i>International Journal of Biological Macromolecules</i> , 1996, 18, 263-274.	7.5	0