Jose Luis Cagide Fajin

List of Publications by Year
in descending order

47	1,431	279701 23	330025 37
papers	citations	h-index	g-index

49	49	49	1713
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Density Functional Theory Study of the Water Dissociation on Platinum Surfaces: General Trends. Journal of Physical Chemistry A, 2014, 118, 5832-5840.	1.1	106
2	Influence of step sites in the molecular mechanism of the water gas shift reaction catalyzed by copper. Journal of Catalysis, 2009, 268, 131-141.	3.1	96
3	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. Journal of Catalysis, 2010, 276, 92-100.	3.1	86
4	Effect of the exchange-correlation potential and of surface relaxation on the description of the H2O dissociation on Cu(111). Journal of Chemical Physics, 2009, 130, 224702.	1.2	84
5	On the theoretical understanding of the unexpected O₂activation by nanoporous gold. Chemical Communications, 2011, 47, 8403-8405.	2.2	73
6	Adsorption of Atomic and Molecular Oxygen on the Au(321) Surface:â€‰ DFT Study. Journal of Physical Chemistry C, 2007, 111, 17311-17321.	1.5	65
7	DFT Study of the CO Oxidation on the Au(321) Surface. Journal of Physical Chemistry C, 2008, 112, 17291-17302.	1.5	65
8	Density functional theory model study of size and structure effects on water dissociation by platinum nanoparticles. Journal of Chemical Physics, 2012, 137, 034701.	1.2	56
9	DFT Study of the Adsorption of <scp>d</scp>-(<scp>l</scp>-)Cysteine on Flat and Chiral Stepped Gold Surfaces. Langmuir, 2013, 29, 8856-8864.	1.6	50
10	Rutheniumâ€“Platinum Catalysts and Direct Methanol Fuel Cells (DMFC): A Review of Theoretical and Experimental Breakthroughs. Catalysts, 2017, 7, 47.	1.6	50
11	Desirability-Based Methods of Multiobjective Optimization and Ranking for Global QSAR Studies. Filtering Safe and Potent Drug Candidates from Combinatorial Libraries. ACS Combinatorial Science, 2008, 10, 897-913.	3.3	46
12	Mechanistic Study of Carbon Monoxide Methanation over Pure and Rhodium- or Ruthenium-Doped Nickel Catalysts. Journal of Physical Chemistry C, 2015, 119, 16537-16551.	1.5	44
13	Generalized BrÃ¸nstedâ€“Evansâ€“Polanyi relationships and descriptors for Oâ€“H bond cleavage of organic molecules on transition metal surfaces. Journal of Catalysis, 2014, 313, 24-33.	3.1	42
14	The Role of Preadsorbed Atomic Hydrogen in the NO Dissociation on a Zigzag Stepped Gold Surface: A DFT Study. Journal of Physical Chemistry C, 2009, 113, 8864-8877.	1.5	39
15	Unraveling the mechanism of the NO reduction by CO on gold based catalysts. Journal of Catalysis, 2012, 289, 11-20.	3.1	36
16	Ionic and radical adsorption on the Au(hkl) surfaces: A DFT study. Surface Science, 2012, 606, 69-77.	0.8	32
17	Water Dissociation on Bimetallic Surfaces: General Trends. Journal of Physical Chemistry C, 2012, 116, 10120-10128.	1.5	32
18	Insights into the Mechanism of Methanol Steam Reforming for Hydrogen Production over Niâ€“Cu-Based Catalysts. ACS Catalysis, 2022, 12, 512-526.	5.5	31

#	Article	IF	Citations
19	Cluster and periodic DFT calculations of adsorption of hydroxyl on the Au(hkl) surfaces. Computational and Theoretical Chemistry, 2010, 946, 43-50.	1.5	28
20	DFT study on the reaction of NO oxidation on a stepped gold surface. Applied Catalysis A: General, 2010, 379, 111-120.	2.2	28
21	Competitive Paths for Methanol Decomposition on Ruthenium: A DFT Study. Journal of Physical Chemistry C, 2015, 119, 27382-27391.	1.5	25
22	Fluorobenzeneâ€“argon ground-state intermolecular potential energy surface. Journal of Chemical Physics, 2004, 120, 8582-8586.	1.2	23
23	DFT study on the reaction of O2 dissociation catalyzed by gold surfaces doped with transition metal atoms. Applied Catalysis A: General, 2013, 458, 90-102.	2.2	23
24	DFT study of the Au(321) surface reconstruction by consecutive deposition of oxygen atoms. Surface Science, 2008, 602, 424-435.	0.8	22
25	On the Need for Spin Polarization in Heterogeneously Catalyzed Reactions on Nonmagnetic Metallic Surfaces. Journal of Chemical Theory and Computation, 2012, 8, 1737-1743.	2.3	21
26	Fischer-Tropsch Synthesis on Multicomponent Catalysts: What Can We Learn from Computer Simulations?. Catalysts, 2015, 5, 3-17.	1.6	20
27	Effect of the Exchange-Correlation Potential on the Transferability of BrÃ¸nstedâ€“Evansâ€“Polanyi Relationships in Heterogeneous Catalysis. Journal of Chemical Theory and Computation, 2016, 12, 2121-2126.	2.3	20
28	A computational study of the interaction of graphene structures with biomolecular units. Physical Chemistry Chemical Physics, 2016, 18, 15312-15321.	1.3	18
29	DFT study on the NO oxidation on a flat gold surface model. Chemical Physics Letters, 2011, 503, 129-133.	1.2	17
30	Effect of van der Waals interactions in the DFT description of self-assembled monolayers of thiols on gold. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	17
31	Accurate intermolecular ground state potential of the Ne-HCl van der Waals complex. Journal of Chemical Physics, 2004, 121, 4599-4604.	1.2	14
32	Water dissociation on multimetallic catalysts. Applied Catalysis B: Environmental, 2017, 218, 199-207.	10.8	14
33	p-Difluorobenzeneâ”Argon Ground State Intermolecular Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2005, 109, 11602-11608.	1.1	12
34	Rotational Structure of Small ⁴He Clusters Seeded with HF, HCl, and HBr Molecules. Journal of Physical Chemistry A, 2007, 111, 12275-12288.	1.1	12
35	Water adsorption and dissociation on the Au(321) stepped surface. Computational and Theoretical Chemistry, 2010, 946, 51-56.	1.5	12
36	Accurate computations of the rovibrational spectrum of the Heâ€“HF van der Waals complex. Molecular Physics, 2006, 104, 1413-1420.	0.8	10

#	Article	IF	Citations
37	Methanol dissociation on bimetallic surfaces: validity of the general BrÃ¸nstedâ€“Evansâ€“Polanyi relationship for Oâ€“H bond cleavage. RSC Advances, 2016, 6, 18695-18702.	1.7	10
38	The Fluorobenzeneâ‹¯Argon S₁ Excited-State Intermolecular Potential Energy Surface. Journal of Physical Chemistry A, 2007, 111, 7876-7881.	1.1	9
39	A DFT study of the NO dissociation on gold surfaces doped with transition metals. Journal of Chemical Physics, 2013, 138, 074701.	1.2	9
40	Catalytic Reactions on Model Gold Surfaces: Effect of Surface Steps and of Surface Doping. Catalysts, 2011, 1, 40-51.	1.6	8
41	Thep-Difluorobenzeneâ‹¯Argon S1Excited State Intermolecular Potential Energy Surface. Journal of Physical Chemistry A, 2006, 110, 13259-13263.	1.1	7
42	First-principles-based kinetic Monte Carlo simulations of CO oxidation on catalytic Au(110) and Ag(110) surfaces. Physical Chemistry Chemical Physics, 2021, 23, 14037-14050.	1.3	7
43	Accurate intermolecular ground state potential of the Heâ€“HCl van der Waals complex. Chemical Physics Letters, 2006, 419, 55-58.	1.2	6
44	Implicit solvent effects in the determination of BrÃ¸nstedâ€“Evansâ€“Polanyi relationships for heterogeneously catalyzed reactions. Physical Chemistry Chemical Physics, 2019, 21, 17687-17695.	1.3	4
45	How reliable is the ReaxFF potential for describing the structure of alkanethiols on gold? A molecular dynamics study. International Journal of Modeling, Simulation, and Scientific Computing, 2014, 05, 1441011.	0.9	1
46	Prediction of metallic nanotube reactivity for H2O activation. Physical Chemistry Chemical Physics, 2017, 19, 19188-19195.	1.3	1
47	N2O Hydrogenation on Silver Doped Gold Catalysts, a DFT Study. Nanomaterials, 2022, 12, 394.	1.9	0