Jose Luis Cagide Fajin

List of Publications by Year in Descending Order

46 papers	1,216 citations	21 h-index	34 g-index
49 ext. papers	1,312 ext. citations	4.5 avg, IF	4.53 L-index

#	Paper	IF	Citations
46	Insights into the Mechanism of Methanol Steam Reforming for Hydrogen Production over Ni□Cu-Based Catalysts. *ACS Catalysis*, **2022**, 12, 512-526	13.1	2
45	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	3.6	1
44	Implicit solvent effects in the determination of Br□sted-Evans-Polanyi relationships for heterogeneously catalyzed reactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 17687-17695	3.6	3
43	Water dissociation on multimetallic catalysts. *Applied Catalysis B: Environmental*, **2017**, 218, 199-207	21.8	11
42	Prediction of metallic nanotube reactivity for HO activation. *Physical Chemistry Chemical Physics*, **2017**, 19, 19188-19195	3.6	1
41	Ruthenium□Platinum Catalysts and Direct Methanol Fuel Cells (DMFC): A Review of Theoretical and Experimental Breakthroughs. *Catalysts*, **2017**, 7, 47	4	36
40	Methanol dissociation on bimetallic surfaces: validity of the general Br□sted□Evans□Polanyi relationship for O□H bond cleavage. *RSC Advances*, **2016**, 6, 18695-18702	3.7	10
39	A computational study of the interaction of graphene structures with biomolecular units. *Physical Chemistry Chemical Physics*, **2016**, 18, 15312-21	3.6	14
38	Effect of the Exchange-Correlation Potential on the Transferability of Br□sted-Evans-Polanyi Relationships in Heterogeneous Catalysis. *Journal of Chemical Theory and Computation*, **2016**, 12, 2121-6	6.4	15
37	Mechanistic Study of Carbon Monoxide Methanation over Pure and Rhodium- or Ruthenium-Doped Nickel Catalysts. *Journal of Physical Chemistry C*, **2015**, 119, 16537-16551	3.8	37
36	Competitive Paths for Methanol Decomposition on Ruthenium: A DFT Study. *Journal of Physical Chemistry C*, **2015**, 119, 27382-27391	3.8	17
35	Effect of van der Waals interactions in the DFT description of self-assembled monolayers of thiols on gold. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	15
34	Fischer-Tropsch Synthesis on Multicomponent Catalysts: What Can We Learn from Computer Simulations?. *Catalysts*, **2015**, 5, 3-17	4	18
33	Generalized Br□sted□Evans□Polanyi relationships and descriptors for O□H bond cleavage of organic molecules on transition metal surfaces. *Journal of Catalysis*, **2014**, 313, 24-33	7.3	39
32	Density functional theory study of the water dissociation on platinum surfaces: general trends. *Journal of Physical Chemistry A*, **2014**, 118, 5832-40	2.8	82
31	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	0.8	1
30	DFT study of the adsorption of D-(L-)cysteine on flat and chiral stepped gold surfaces. *Langmuir*, **2013**, 29, 8856-64	4	44

29	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	5.1	23
28	A DFT study of the NO dissociation on gold surfaces doped with transition metals. *Journal of Chemical Physics*, **2013**, 138, 074701	3.9	9
27	Unraveling the mechanism of the NO reduction by CO on gold based catalysts. *Journal of Catalysis*, **2012**, 289, 11-20	7.3	29
26	Density functional theory model study of size and structure effects on water dissociation by platinum nanoparticles. *Journal of Chemical Physics*, **2012**, 137, 034701	3.9	49
25	On the Need for Spin Polarization in Heterogeneously Catalyzed Reactions on Nonmagnetic Metallic Surfaces. *Journal of Chemical Theory and Computation*, **2012**, 8, 1737-43	6.4	19
24	Ionic and radical adsorption on the Au(hkl) surfaces: A DFT study. *Surface Science*, **2012**, 606, 69-77	1.8	29
23	Water Dissociation on Bimetallic Surfaces: General Trends. *Journal of Physical Chemistry C*, **2012**, 116, 10120-10128	3.8	26
22	On the theoretical understanding of the unexpected O2 activation by nanoporous gold. *Chemical Communications*, **2011**, 47, 8403-5	5.8	60
21	Catalytic Reactions on Model Gold Surfaces: Effect of Surface Steps and of Surface Doping. *Catalysts*, **2011**, 1, 40-51	4	4
20	DFT study on the NO oxidation on a flat gold surface model. *Chemical Physics Letters*, **2011**, 503, 129-133	2.5	14
19	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. *Journal of Catalysis*, **2010**, 276, 92-100	7.3	74
18	Water adsorption and dissociation on the Au(321) stepped surface. *Computational and Theoretical Chemistry*, **2010**, 946, 51-56		11
17	Cluster and periodic DFT calculations of adsorption of hydroxyl on the Au(h k l) surfaces. *Computational and Theoretical Chemistry*, **2010**, 946, 43-50		24
16	DFT study on the reaction of NO oxidation on a stepped gold surface. *Applied Catalysis A: General*, **2010**, 379, 111-120	5.1	27
15	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
14	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
13	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	3.8	38
12	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		40

11	DFT Study of the CO Oxidation on the Au(321) Surface. *Journal of Physical Chemistry C*, **2008**, 112, 17291-17302	3.8	61
10	DFT study of the Au(321) surface reconstruction by consecutive deposition of oxygen atoms. *Surface Science*, **2008**, 602, 424-435	1.8	21
9	Rotational structure of small 4He clusters seeded with HF, HCl, and HBr molecules. *Journal of Physical Chemistry A*, **2007**, 111, 12275-88	2.8	10
8	Adsorption of Atomic and Molecular Oxygen on the Au(321) Surface: DFT Study. *Journal of Physical Chemistry C*, **2007**, 111, 17311-17321	3.8	59
7	The fluorobenzene-argon S(1) excited-state intermolecular potential energy surface. *Journal of Physical Chemistry A*, **2007**, 111, 7876-81	2.8	8
6	Accurate computations of the rovibrational spectrum of the He–HF van der Waals complex. *Molecular Physics*, **2006**, 104, 1413-1420	1.7	9
5	The p-difluorobenzene-argon S1 excited state intermolecular potential energy surface. *Journal of Physical Chemistry A*, **2006**, 110, 13259-63	2.8	6
4	Accurate intermolecular ground state potential of the He–HCl van der Waals complex. *Chemical Physics Letters*, **2006**, 419, 55-58	2.5	6
3	p-Difluorobenzene-argon ground state intermolecular potential energy surface. *Journal of Physical Chemistry A*, **2005**, 109, 11602-8	2.8	11
2	Accurate intermolecular ground state potential of the Ne-HCl van der Waals complex. *Journal of Chemical Physics*, **2004**, 121, 4599-604	3.9	13
1	Fluorobenzene-argon ground-state intermolecular potential energy surface. *Journal of Chemical Physics*, **2004**, 120, 8582-6	3.9	23