David Loffreda

List of Publications by Year
in descending order

53	3,927	186254 28	155644 55
papers	citations	h-index	g-index

60	60	60	4400
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Finding optimal surface sites on heterogeneous catalysts by counting nearest neighbors. Science, 2015, 350, 185-189.	12.6	725
2	Introducing structural sensitivity into adsorptionâ€“energy scaling relations by means of coordination numbers. Nature Chemistry, 2015, 7, 403-410.	13.6	600
3	Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers. Angewandte Chemie - International Edition, 2014, 53, 8316-8319.	13.8	366
4	Performance and degradation of Proton Exchange Membrane Fuel Cells: State of the art in modeling from atomistic to system scale. Journal of Power Sources, 2016, 304, 207-233.	7.8	180
5	Why conclusions from platinum model surfaces do not necessarily lead to enhanced nanoparticle catalysts for the oxygen reduction reaction. Chemical Science, 2017, 8, 2283-2289.	7.4	173
6	Theoretical Evidence of PtSn Alloy Efficiency for CO Oxidation. Journal of the American Chemical Society, 2006, 128, 9129-9136.	13.7	147
7	Vibrational frequency and chemisorption site: a DFT-periodic study of NO on Pd (111) and Rh (111) surfaces. Chemical Physics Letters, 1998, 291, 15-23.	2.6	139
8	Fast Prediction of Selectivity in Heterogeneous Catalysis from Extended BrÃ¸nstedâ€“Evansâ€“Polanyi Relations: A Theoretical Insight. Angewandte Chemie - International Edition, 2009, 48, 8978-8980.	13.8	126
9	Chemoâˆ’Regioselectivity in Heterogeneous Catalysis:Â Competitive Routes for CO and CC Hydrogenations from a Theoretical Approach. Journal of the American Chemical Society, 2006, 128, 1316-1323.	13.7	122
10	Catalytic Hydrogenation of Unsaturated Aldehydes on Pt(111): Understanding the Selectivity from First-Principles Calculations. Angewandte Chemie - International Edition, 2005, 44, 5279-5282.	13.8	113
11	Theoretical insight of adsorption thermodynamics of multifunctional molecules on metal surfaces. Surface Science, 2006, 600, 2103-2112.	1.9	76
12	Coverage Dependent Adsorption of Acrolein on Pt(111) from a Combination of First Principle Theory and HREELS Study. Journal of Physical Chemistry B, 2004, 108, 9085-9093.	2.6	75
13	A multiscale theoretical methodology for the calculation of electrochemical observables from ab initio data: Application to the oxygen reduction reaction in a Pt(111)-based polymer electrolyte membrane fuel cell. Electrochimica Acta, 2011, 56, 10842-10856.	5.2	68
14	Catalytic consequences of ultrafine Pt clusters supported on SrTiO3 for photocatalytic overall water splitting. Journal of Catalysis, 2019, 376, 180-190.	6.2	67
15	Breaking the NO bond on Rh, Pd, and Pd3Mn alloy (100) surfaces: A quantum chemical comparison of reaction paths. Journal of Chemical Physics, 2001, 115, 8101-8111.	3.0	61
16	Affordable Estimation of Solvation Contributions to the Adsorption Energies of Oxygenates on Metal Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 5578-5582.	3.1	54
17	Highly selective hydrogenation of butadiene on Pt/Sn alloy elucidated by first-principles calculations. Journal of Catalysis, 2010, 275, 129-139.	6.2	51
18	Adsorption of Î±,Î²-Unsaturated Aldehydes on Pt(111) and Ptâˆ’Sn Alloys: II. Crotonaldehyde. Journal of Physical Chemistry C, 2009, 113, 13947-13967.	3.1	48

#	Article	IF	Citations
19	Promoter Effect of Early Stage Grown Surface Oxides: A Near-Ambient-Pressure XPS Study of CO Oxidation on PtSn Bimetallics. Journal of Physical Chemistry Letters, 2012, 3, 3707-3714.	4.6	43
20	Theoretical elucidation of the selectivity changes for the hydrogenation of unsaturated aldehydes on Pt(111). Journal of Catalysis, 2009, 265, 35-42.	6.2	41
21	Understanding Adsorption-Induced Effects on Platinum Nanoparticles: An Energy-Decomposition Analysis. Journal of Physical Chemistry Letters, 2014, 5, 3120-3124.	4.6	37
22	Adsorption and Vibrations of Î±,Î²-Unsaturated Aldehydes on Pure Pt and Ptâ˜Sn Alloy (111) Surfaces I. Prenal. Journal of Physical Chemistry C, 2008, 112, 3701-3718.	3.1	36
23	Adsorption and Vibrations of Î±,Î²-Unsaturated Aldehydes on Pt(111) and Ptâ˜Sn Alloy (111) Surfaces. 3. Adsorption Energy vs Adsorption Strength. Journal of Physical Chemistry C, 2010, 114, 1073-1084.	3.1	35
24	How Surface Hydroxyls Enhance MgO Reactivity in Basic Catalysis: The Case of Methylbutynol Conversion. ACS Catalysis, 2014, 4, 4004-4014.	11.2	34
25	Adsorption thermodynamics of acrolein on Pt (111) in realistic temperature and pressure from first-principle calculations. Chemical Physics Letters, 2005, 405, 434-439.	2.6	32
26	Heterogeneous Catalytic Hydrogenation: Is Double Bond/Surface Coordination Necessary?. Journal of Physical Chemistry Letters, 2010, 1, 323-326.	4.6	31
27	Metalâ€“support interaction effects on chemoâ€“regioselectivity: Hydrogenation of crotonaldehyde on Pt 13 /CeO 2 (1 1 1). Journal of Catalysis, 2016, 334, 68-78.	6.2	31
28	Tuning catalytic reactivity on metal surfaces: Insights from DFT. Journal of Catalysis, 2013, 308, 374-385.	6.2	29
29	First-Principles Study of CO Adsorption and Vibration on Au Surfaces. Journal of Physical Chemistry B, 2005, 109, 9596-9603.	2.6	28
30	Determination of the crotonaldehyde structures on Pt and PtSn surface alloys from a combined experimental and theoretical study. Chemical Physics Letters, 2006, 433, 188-192.	2.6	27
31	Adsorption of Simple Alkenes on Pt(111) and Ptâ˜Sn Surface Alloys: Bond Strength versus Heat of Adsorption. Journal of Physical Chemistry C, 2008, 112, 14693-14695.	3.1	25
32	Capturing Solvation Effects at a Liquid/Nanoparticle Interface by Ab Initio Molecular Dynamics: Pt₂₀₁ Immersed in Water. Small, 2016, 12, 5312-5319.	10.0	25
33	Interplay between Reaction Mechanism and Hydroxyl Species for Water Formation on Pt(111). ACS Catalysis, 2015, 5, 1068-1077.	11.2	24
34	Coverage-dependent thermodynamic analysis of the formation of water and hydrogen peroxide on a platinum model catalyst. Physical Chemistry Chemical Physics, 2015, 17, 11392-11400.	2.8	20
35	Mediatory role of tin in the catalytic performance of tailored platinumâ€“tin alloy surfaces for carbon monoxide oxidation. Journal of Catalysis, 2010, 273, 211-220.	6.2	15
36	A Water Solvation Shell Can Transform Gold Metastable Nanoparticles in the Fluxional Regime. Journal of Physical Chemistry Letters, 2019, 10, 1092-1098.	4.6	14

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37	Growth of a Pt film on non-reduced ceria: A density functional theory study. Journal of Chemical Physics, 2012, 136, 044705.	3.0	13
38	Revealing Size Dependent Structural Transitions in Supported Gold Nanoparticles in Hydrogen at Atmospheric Pressure. Small, 2021, 17, e2104571.	10.0	13
39	Diffusion Kinetics of Gold and Copper Atoms on Pristine and Reduced Rutile TiO₂ (110) Surfaces. Journal of Physical Chemistry C, 2018, 122, 3824-3837.	3.1	12
40	Support Effects Examined by a Comparative Theoretical Study of Au, Cu, and CuAu Nanoclusters on Rutile and Anatase Surfaces. Journal of Physical Chemistry C, 2019, 123, 4892-4902.	3.1	11
41	Effect of the Ligand Binding Strength on the Morphology of Functionalized Gold Nanoparticles. Journal of Physical Chemistry Letters, 2020, 11, 2717-2723.	4.6	11
42	Importance of Defective and Nonsymmetric Structures in Silver Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 3705-3711.	4.6	11
43	Structural Identification of Conjugated Molecules on Metal Surfaces by Means of Soft Vibrations. Angewandte Chemie - International Edition, 2006, 45, 6537-6540.	13.8	10
44	Catalytic activation of a non-noble intermetallic surface through nanostructuration under hydrogenation conditions revealed by atomistic thermodynamics. Journal of Materials Chemistry A, 2020, 8, 7422-7431.	10.3	10
45	Mechanistic and spectroscopic identification of initial reaction intermediates for prenal decomposition on a platinum model catalyst. Physical Chemistry Chemical Physics, 2011, 13, 6000.	2.8	9
46	How Does the Surface Structure of Ptâ€“Ni Alloys Control Water and Hydrogen Peroxide Formation?. ACS Catalysis, 2016, 6, 5641-5650.	11.2	9
47	Nature of adhesion of condensed organic films on platinum by first-principles simulations. Physical Chemistry Chemical Physics, 2011, 13, 11827.	2.8	8
48	Monte Carlo simulation of free radical production under keV photon irradiation of gold nanoparticle aqueous solution. Part I: Global primary chemical boost. Radiation Physics and Chemistry, 2020, 172, 108790.	2.8	6
49	Coordination of Ethylamine on Small Silver Clusters: Structural and Topological (ELF, QTAIM) Analyses. Inorganic Chemistry, 2022, 61, 7274-7285.	4.0	6
50	Promoter effect of hydration on the nucleation of nanoparticles: direct observation for gold and copper on rutile TiO₂(110). Nanoscale, 2016, 8, 16475-16485.	5.6	5
51	Titelbild: Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers (Angew. Chem. 32/2014). Angewandte Chemie, 2014, 126, 8393-8393.	2.0	1
52	Cover Picture: Catalytic Hydrogenation of Unsaturated Aldehydes on Pt(111): Understanding the Selectivity from First-Principles Calculations (Angew. Chem. Int. Ed. 33/2005). Angewandte Chemie - International Edition, 2005, 44, 5151-5151.	13.8	0
53	Cover Picture: Fast Prediction of Selectivity in Heterogeneous Catalysis from Extended BrÃ¸nsted-Evans-Polanyi Relations: A Theoretical Insight (Angew. Chem. Int. Ed. 47/2009). Angewandte Chemie - International Edition, 2009, 48, 8797-8797.	13.8	0