# David Loffreda

List of Publications by Year
in descending order



| 53 | 3,927 | 186265 28 | 155660 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: Pt<sub>201</sub> 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 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 TiO<sub>2</sub> (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 TiO<sub>2</sub>(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 |