Sergio Posada-PÃ©rez

List of Publications by Year
in descending order

17 papers	716 citations	687335 13 h-index	1058452 14 g-index
18 all docs	18 docs citations	18 times ranked	807 citing authors

#	Article	IF	Citations
1	The bending machine: CO₂ activation and hydrogenation on Î´-MoC(001) and Î²-Mo₂C(001) surfaces. Physical Chemistry Chemical Physics, 2014, 16, 14912-14921.	2.8	175
2	Highly Active Au/Î´-MoC and Cu/Î´-MoC Catalysts for the Conversion of CO₂: The Metal/C Ratio as a Key Factor Defining Activity, Selectivity, and Stability. Journal of the American Chemical Society, 2016, 138, 8269-8278.	13.7	140
3	The conversion of CO₂ to methanol on orthorhombic Î²-Mo₂C and Cu/Î²-Mo₂C catalysts: mechanism for admetal induced change in the selectivity and activity. Catalysis Science and Technology, 2016, 6, 6766-6777.	4.1	101
4	Fundamentals of Methanol Synthesis on Metal Carbide Based Catalysts: Activation of CO2 and H2. Topics in Catalysis, 2015, 58, 159-173.	2.8	64
5	Adsorption and dissociation of molecular hydrogen on orthorhombic Î²-Mo2C and cubic Î´-MoC (001) surfaces. Surface Science, 2017, 656, 24-32.	1.9	50
6	Highly active Au/Î´-MoC and Au/Î²-Mo₂C catalysts for the low-temperature water gas shift reaction: effects of the carbide metal/carbon ratio on the catalyst performance. Catalysis Science and Technology, 2017, 7, 5332-5342.	4.1	39
7	Kinetic Monte Carlo Simulations Unveil Synergic Effects at Work on Bifunctional Catalysts. ACS Catalysis, 2019, 9, 9117-9126.	11.2	30
8	Structure and electronic properties of Cu nanoclusters supported on Mo2C(001) and MoC(001) surfaces. Journal of Chemical Physics, 2015, 143, 114704.	3.0	25
9	Exploring cocatalyst type effect on the Zieglerâ€“Natta catalyzed ethylene polymerizations: experimental and DFT studies. Journal of Polymer Research, 2022, 29, .	2.4	19
10	Methane capture at room temperature: adsorption on cubic Î´-MoC and orthorhombic Î²-Mo₂C molybdenum carbide (001) surfaces. RSC Advances, 2015, 5, 33737-33746.	3.6	18
11	The importance of the bite angle of metal(III) salen catalysts in the sequestration of CO2 with epoxides in mild conditions. Green Chemical Engineering, 2022, 3, 180-187.	6.3	18
12	CO₂ interaction with violarite (FeNi₂S₄) surfaces: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2018, 20, 20439-20446.	2.8	15
13	Influence of Stacking on H⁺ Intercalation in Layered ACoO₂ (A =) Tj ETQq1 1 0.784314 rgBT O Investigation. Chemistry of Materials, 2021, 33, 6942-6954.	6.7	15
14	Effect of Aqueous Electrolytes on LiCoO₂ Surfaces: Role of Proton Adsorption on Oxygen Vacancy Formation. Journal of Physical Chemistry C, 2022, 126, 110-119.	3.1	7
15	The Importance of Li-Ion Nature and Stacking in Layered Cathode Materials for Aqueous Ion Batteries: From Bulk to Surface Models. ECS Meeting Abstracts, 2021, MA2021-01, 99-99.	0.0	0
16	Are Protons Involve in the Fading Capacity in Li Ion Aqueous Batteries? Shedding Light By Means of First Principle Computations. ECS Meeting Abstracts, 2020, MA2020-01, 223-223.	0.0	0
17	Shedding Light about the Role of Proton Intercalation in Layered Cathode Materials By Means of First Principle Computations. ECS Meeting Abstracts, 2020, MA2020-02, 68-68.	0.0	0