David Samuel Rivera Rocabado

List of Publications by Year
in descending order

12 papers	67 citations	1478505 6 h-index	1588992 8 g-index
12 all docs	12 docs citations	12 times ranked	49 citing authors

#	Article	IF	Citations
1	Hydrogen/Deuterium Transfer from Anisole to Methoxy Radicals: A Theoretical Study of a Deuterium-Labeled Drug Model. Journal of Physical Chemistry A, 2022, 126, 155-163.	2.5	3
2	Uncovering the Mechanism of the Hydrogen Poisoning on Ru Nanoparticles via Density Functional Theory Calculations. Catalysts, 2022, 12, 331.	3.5	7
3	Hydrogen absorption and diffusion behaviors in cube-shaped palladium nanoparticles revealed by ambient-pressure X-ray photoelectron spectroscopy. Applied Surface Science, 2022, 587, 152797.	6.1	7
4	First-Principles Calculations of Stability, Electronic Structure, and Sorption Properties of Nanoparticle Systems. Journal of Computer Chemistry Japan, 2021, 20, 23-47.	0.1	0
5	Density Functional Theory and Machine Learning Description and Prediction of Oxygen Atom Chemisorption on Platinum Surfaces and Nanoparticles. ACS Omega, 2021, 6, 17424-17432.	3.5	9
6	Adsorption States of N₂/H₂ Activated on Ru Nanoparticles Uncovered by Modulationâ€“Excitation Infrared Spectroscopy and Density Functional Theory Calculations. ACS Nano, 2021, 15, 20079-20086.	14.6	10
7	Electronic structure and phase stability of Pt3M (MÂ=ÂCo, Ni, and Cu) bimetallic nanoparticles. Computational Materials Science, 2020, 184, 109874.	3.0	9
8	The effect of SnO2(110) supports on the geometrical and electronic properties of platinum nanoparticles. SN Applied Sciences, 2019, 1, 1.	2.9	13
9	Theoretical Approach to the Sulfidation of the BaTiO₃(001) Surfaces and Its Effect on the H₂ Oxidation Reaction and CH₄ Sequential Dissociation. Journal of Physical Chemistry C, 2018, 122, 1437-1446.	3.1	3
10	First-Principles Study on Alloy Nanoparticles for Polymer Electrolyte Fuel Cell Catalyst. ECS Transactions, 2016, 75, 717-721.	0.5	3
11	Theoretical Study of Inorganic Carbonaceous Species Reaction with the Surfaces of BaTiO3(001). ECS Transactions, 2015, 68, 3177-3185.	0.5	1
12	Density Functional Theory Study on the Catalytic Properties of BaTiO3 as Solid Oxide Fuel Cell Anode. ECS Transactions, 2013, 57, 2723-2732.	0.5	2