

# Al Rey C Villagracia

## List of Publications by Year in descending order

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Version: 2024-02-01

40  
papers

635  
citations

623734

14  
h-index

610901

24  
g-index

42  
all docs

42  
docs citations

42  
times ranked

661  
citing authors

#	ARTICLE	IF	CITATIONS
1	Hydrogen adsorption on pristine, defected, and 3d-block transition metal-doped penta-graphene. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 12157-12166.	7.1	78
2	Characterization of nanocellulose recovery from <i>Elaeis guineensis</i> frond for sustainable development. <i>Clean Technologies and Environmental Policy</i> , 2016, 18, 2503-2512.	4.1	63
3	Ca and K decorated germanene as hydrogen storage: An ab initio study. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 4393-4400.	7.1	54
4	Biomass-derived cellulose nanofibrils membrane from rice straw as sustainable separator for high performance supercapacitor. <i>Industrial Crops and Products</i> , 2021, 170, 113694.	5.2	54
5	Microwave drying characteristics of microalgae ( <i>Chlorella vulgaris</i> ) for biofuel production. <i>Clean Technologies and Environmental Policy</i> , 2016, 18, 2441-2451.	4.1	42
6	Theoretical Investigation on Single-Wall Carbon Nanotubes Doped with Nitrogen, Pyridine-Like Nitrogen Defects, and Transition Metal Atoms. <i>Journal of Nanomaterials</i> , 2012, 2012, 1-14.	2.7	40
7	Unveiling the physicochemical properties of natural <i>Citrus aurantifolia</i> crosslinked tapioca starch/nanocellulose bionanocomposites. <i>Industrial Crops and Products</i> , 2019, 139, 111548.	5.2	36
8	Theoretical Investigation on the Solubilization in Water of Functionalized Single-Wall Carbon Nanotubes. <i>Journal of Nanotechnology</i> , 2012, 2012, 1-6.	3.4	24
9	DFT Investigation on the Electronic and Water Adsorption Properties of Pristine and N-Doped TiO <sub>2</sub> Nanotubes for Photocatalytic Water Splitting Applications. <i>Journal of Electronic Materials</i> , 2017, 46, 3592-3602.	2.2	24
10	Ab initio study on hydrogen interaction with calcium decorated silicon carbide nanotube. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 11452-11460.	7.1	21
11	Investigation of reverse ionic diffusion in forward-osmosis-aided dewatering of microalgae: A molecular dynamics study. <i>Bioresource Technology</i> , 2019, 279, 181-188.	9.6	21
12	Swelling behavior and chemical stability of chitosan/nanocellulose biocomposites. <i>Polymer Composites</i> , 2018, 39, E561.	4.6	19
13	H <sub>2</sub> adsorption on K decorated germanene surface: anab-initioinvestigation. <i>Materials Research Express</i> , 2016, 3, 115015.	1.6	16
14	A Review on Nanocellulose and Its Application in Supercapacitors. <i>Macromolecular Materials and Engineering</i> , 2021, 306, 2100556.	3.6	16
15	Revealing the Water Resistance, Thermal and Biodegradation Properties of <i>Citrus aurantifolia</i> Crosslinked Tapioca Starch/Nanocellulose Bionanocomposites. <i>Journal of Polymers and the Environment</i> , 2020, 28, 3256-3269.	5.0	15
16	Utilization of Modified Palm Kernel Shell for Biocomposites Production. <i>Key Engineering Materials</i> , 0, 700, 60-69.	0.4	13
17	Effects of polypropylene methyl polyhedral oligomeric silsesquioxanes and polypropylene-grafted maleic anhydride compatibilizers on the properties of palm kernel shell reinforced polypropylene biocomposites. <i>Polimeros</i> , 2016, 26, 228-235.	0.7	12
18	Effects of salinity on the CO <sub>2</sub> permeation across lipid bilayer for microalgae biofixation: a molecular dynamics study. <i>Journal of Applied Phycology</i> , 2018, 30, 55-61.	2.8	12

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19	First principles study of H <sub>2</sub> adsorption on Ni-decorated silicene. Materials Research Express, 2019, 6, 055509.	1.6	12
20	Comparative Study of Microcelluloses Isolated From Two Different Biomasses with Commercial Cellulose. BioResources, 2016, 11, .	1.0	8
21	First Principles Investigation on H <sub>2</sub> Adsorption on the Pristine 2-Dimensional Hexagonal Aluminum. IOP Conference Series: Earth and Environmental Science, 2019, 268, 012135.	0.3	8
22	Negative differential resistance in polymer tunnel diodes using atomic layer deposited, TiO <sub>2</sub> tunneling barriers at various deposition temperatures. Organic Electronics, 2017, 47, 228-234.	2.6	7
23	Hydrogen adsorption on calcium, potassium, and magnesium-decorations aluminene using density functional theory. International Journal of Hydrogen Energy, 2021, 46, 16676-16684.	7.1	7
24	Chemical reactivity and bioactivity properties of pyrazinamide analogs of acetylsalicylic acid and salicylic acid using conceptual density functional theory. Heliyon, 2020, 6, e04239.	3.2	6
25	Effect of compatibiliser on the accelerated weathering performance of polypropylene-silica nanocomposites. Materials Research Innovations, 2014, 18, S6-433-S6-438.	2.3	5
26	Tailoring the Chemical and Structural Properties of Graphene Oxide Nanoplatelets Synthesised at Room Temperature with Different Processing Times. Journal of Physical Science, 2017, 28, 19-40.	0.9	5
27	Molecular dynamics study on the effects of varying temperature and pressure on phosphatidylcholine lipids for microalgae drying. , 2014, , .		3
28	Density Functional Theory-based modeling and calculations of a polyamide molecular unit for studying forward-osmosis-dewatering of microalgae. , 2018, , .		3
29	Investigation of the drying characteristics of microalgae using microwave irradiation. , 2015, , .		2
30	A comparative study of green composites based on tapioca starch and celluloses. AIP Conference Proceedings, 2017, , .	0.4	2
31	Co <sub>2</sub> transport from flue gas emission across the lipid membrane for microalgae biofixation. , 2017, , .		2
32	Investigation on water adsorption on 3-crosslinked circular polyacrylamide membrane using ab initio, molecular dynamics and monte carlo calculations for dewatering microalgae. IOP Conference Series: Earth and Environmental Science, 2019, 268, 012144.	0.3	2
33	Course-grained molecular dynamics investigation on the effects of uniform electric field on DPPC lipid bilayer: With and without vacuum space. , 2017, , .		0
34	Effect of structural and dynamical properties of lipid bilayer on water permeation studied using course-grained molecular dynamics simulation. , 2017, , .		0
35	Effect of Mesoporous Nanoparticles from LCD Glass Panels Waste toward Polypropylene Based Hybrid Composites. , 2018, , .		0
36	First Principles Investigation on the Elastic Properties of Mg, Ca, K-decorated Planar Aluminene. , 2019, , .		0

#	ARTICLE	IF	CITATIONS
37	Elastic Properties of B, C, N-decorated on Planar Aluminene using Density Functional Theory. , 2019, , .		0
38	H2O Absorptivity on a Fully 4-crosslinked Polyacrylamide Membrane via Density Functional Theory and Monte Carlo Calculations for Draw Solution Recovery in Forward Osmosis. , 2019, , .		0
39	Unit operations applied to drying microalgal biomass. , 2022, , 213-224.		0
40	First principles investigation on the hydrogen adsorption on planar aluminene with boron, carbon, and nitrogen as impurities. Molecular Physics, 0, , .	1.7	0