

Research Article:

1. **B Saini**, R Krishnapriya, M Yadav, R Singhal, and RK Sharma; On the reduction of CO₂ footprint via selective hydrodeoxygenation by ZnO-Ti₃C₂Tx catalyst under solvent-free conditions **Green Chemistry** **2023**, 25, 5470-5482.
2. **B Saini**, M Yadav, SK Jha, R Krishnapriya, P Kang, V Kant, R Singhal, RK Sharma; Highly selective production of bio-jet fuel grade alkanes over Fe/SiO₂-Al₂O₃ solid acid catalyst under solvent-free conditions **RSC Sustainable Energy and Fuels** **2023**, 7, 2568-2581.
3. **B Saini**, R Krishnapriya, D Laishram, MK Singh, R Singhal, S Bandaru, RK Sharma; Impact of gadolinium doping into the frustrated antiferromagnetic lithium manganese oxide spinel, **iScience**, **2023** 26 (1), 105869.
4. **B Saini**, D Laishram, R Krishnapriya, R Singhal, RK Sharma; Role of ZnO in ZnO Nanoflake/Ti₃C₂ MXene Composites in Photocatalytic and Electrocatalytic Hydrogen Evolution, **ACS Applied Nano Materials**, **2022** 5 (7), 9319-9333.
5. U Gupta, M Yadav, **B Saini**; R. Krishnapriya; RK Sharma; FexNiy/ SiO₂-Al₂O₃ catalyzed hydrodeoxygenation of biorenewable platform molecules, **Fuel** **2024**, 360, 130588.
6. G Choudhary, M Yadav, **B Saini**, PR Sharma, S Pandey, V Kant, RK Sharma, Effect of calcination temperature on hydroxyapatite in fluoride removal from groundwater water: Process optimization and kinetic study, **Desalination**, **2024**, 574, 117268.
7. R Singhal, **B Saini**, M Kiehnle-Benitez, T Sadowski, C Broadbridge, J Scanley, PK LeMaire, RK Sharma; Effect of multi-wall carbon nanotubes on electrochemical performances of MnO₂, **AIP Advances**, **2022** 12 (8), 085306.
8. R Krishnapriya, C Nizamudeen, **B Saini**, MS Mozumder, RK Sharma, A-HI Mourad; MOF-derived Co²⁺-doped TiO₂ nanoparticles as photoanodes for dye-sensitized solar cells, **Scientific reports**, **2021** 11 (1), 16265.
9. D Laishram, R Krishnapriya, **B Saini**, U Gupta, VK Soni, RK Sharma; Nickel and cobalt transfigured natural clay: a green catalyst for low-temperature catalytic soot oxidation, **New Journal of Chemistry**, **2021** 45 (32), 14751-14758.
10. D Laishram, D Kumar, V Kant, **B Saini**, KP Shejale, R Krishnapriya, VC Janu, R Singhal, RK Sharma; Activated hollow and solid carbon spheres for enhanced removal efficiency of pharmaceutical pollutants and heavy metals in water, **Water, Air, & Soil Pollution**, **2022** 233 (10), 404.
11. S Ponnada, MS Kiai, DB Gorle, R Venkatachalam, **B Saini**, K Murugavel, A Nowduri, R Singhal, F Marken, AM Kulandainathan, KK Nanda, RK Sharma, RSC Bose; Recent status and challenges in multifunctional electrocatalysis based on 2D MXenes **Catalysis Science & Technology**, **2022**, 12, 4413-4441.

Book Chapters:

1. Krishnapriya, R.; Laishram, D.; **Saini, B.**; Jabeen Fatima, M.; Sharma, R. K., Electrospun Cobalt Based Composites as Anodes for Lithium-Ion Batteries. **Electrospinning for Advanced Energy Storage Applications** **2021**, 319-344.
2. Laishram, D.; Kumar, D.; Shejale, K. P.; **Saini, B.**; Harikrishna; Krishnapriya, R.; Sharma, R. K., 2D Transition Metal Carbides (MXenes) for Applications in Electrocatalysis. **Heterogeneous Nanocatalysis for Energy and Environmental Sustainability** **2022**, 1, 165-198.

Annexure A

Materials and Methods

A.1 Reagents

To conduct the experiments and reactions the following list of chemicals were procured from various sources and listed below:

Chemicals/Reagents	Make/Source
Absolute ethanol	Changshu Hongsheng Fine Chemical Co., Ltd, China
Aluminum acetylacetonate	Sigma Aldrich
p-Benzoquinone	Sigma Aldrich
Ciprofloxacin	Sigma Aldrich
Triethanolamine	Sigma Aldrich
<i>Tert</i> -butanol	Sigma Aldrich
Manganese acetate	Alfa Aeser
Methyl orange	Acros
Methyl oleate	Sigma Aldrich
Methylene blue	SRL
Cresol red	Sigma
Lithium acetate	Alfa Aeser
Gadolinium Acetate Tetrahydrate	Alfa Aeser
Tetraethyl orthosilicate	Sigma Aldrich
Iron (III) nitrate nonahydrate	Alfa Aeser
2-ethylhexanoic acid	Sigma
Ethanol	Shangzu, China
Ethylenediamine	Sigma Aldrich
sodium hydroxide	Across Organics
Tetraethyl orthosilicate	Sigma Aldrich
Titanium aluminum carbide	Nanoshel
Ibuprofen	Sigma Aldrich
Hydrofluoric acid	Sigma Aldrich
Oleyl amine	Sigma Aldrich
Nitric acid	Fischer Scientific
1-Octadecene	Sigma Aldrich
zinc acetate dehydrate	Across Organics

A.2 Instrumentation Techniques

The synthesized ZnO-Ti₃C₂ composites were analyzed by X-ray diffraction (XRD) techniques using a D8 Advance X-ray diffractometer (Bruker, U.S.A.), with Cu K α radiation ($\lambda = 1.54 \text{ \AA}$) at an accelerating voltage of 45 kV and tube current of 40 mA to scan the diffraction angle range of 5 to 80°. The International Centre for Diffraction Data (ICDD) database's standard

patterns were used to carry out the phase identification. A Brunauer-Emmet-Teller (BET) method for N₂ adsorption-desorption was performed to measure the specific surface area to understand the effect in photocatalysis and electrocatalysis applications using the Quantachrome Autosorb iQ3 instrument. The as-synthesized ZnO Ti₃C₂ was subjected to degassing for 120 min at 150 °C to remove all of the impurities from the layers. A Gaussian function was used to fit the acquired spectra in order to identify the surface composition and chemical states using an Omicron Nanotechnology (Oxford Instruments) X-ray photoelectron spectroscope (XPS) equipment with monochromatic Al K α radiation. The standard C 1s peak at 284.1 eV was used as the reference point for the peak adjustment. Thermogravimetric (TGA) analysis was carried out on a simultaneous thermal analyzer (STA) from PerkinElmer at 2.5 bar of gas pressure from room temperature to 450 °C with a heating rate of 10 °C/min under an N₂ atmosphere. The high-performance liquid chromatography 515 pump was equipped using a Waters 2489 system and C18 column (250 mm $\times$ 4.6 mm, 5 μ m) system with a mobile phase of 60:40 acetonitrile-water at a 1 mL min⁻¹ flow rate. The pH of the electrode solution and dye solution was measured using Oakton PH 2700. The surface morphology and component distribution were obtained through scanning electron microscopy techniques (EVO 18 Zeiss) at an accelerating voltage of 20 kV and atomic force microscopy (XE-70, Park System). The electrocatalyst performances and electrochemical impedance spectroscopy (EIS) were measured using a CHI660E-CH Instruments Inc. electrochemical workstation. A PET Photo Emission Tech SS50AAA solar simulator was used as a light source to get one sun irradiation for dye degradation experiments. The functional groups of the Fe-loaded SiO₂-Al₂O₃ catalyst were analyzed by Fourier-transform infrared spectroscopy (FTIR) between 4000 and 400 cm⁻¹ with a resolution of 4 cm⁻¹ and 32 using a Jasco FT/IR-4100. A chemisorption analyzer (Altamira instruments, AMI-300) fitted with a thermal conductivity detector (TCD) was used to carry out the temperature-programmed reduction of hydrogen (H₂-TPR) and ammonia (NH₃-TPD). The samples for H₂-TPR were preheated at 150 °C for 1 h at a rate of 10 °C per minute in a helium environment and then allowed to cool to ambient temperature. To record the TPR spectra, the temperature was raised to 900 °C at a rate of 10 °C per minute for 30 minutes while using a mixture of H₂ (5%) and He (95%) as a reducing agent. In the NH₃-TPD program, pretreatment was done with helium gas at a rate of 10 °C min⁻¹ at 200 °C for 1 h. After that, the adsorption of NH₃ was monitored for 60 min at 100 °C. The sample was purged with helium for 2 h to remove the physically adsorbed NH₃. The NH₃-TPD profile was recorded in the range of 100–900 °C. A PerkinElmer Elite-5 capillary column with a 30 m length, 0.25 mm inner diameter, 0.10 μ m thickness, and a temperature range of -60 to 325/350 °C was used for the GC analysis utilizing a PerkinElmer Clarus 580 gas chromatograph. An 11.2 Tesla Bruker ASCENDTM 500WB NMR spectrometer was used to measure ¹H and ¹³C nuclear magnetic resonance (NMR) spectra at 500 MHz. A single pulse sequence was used to record the spectra, with a 90° pulse duration of 1 s and a 1 μ s inter-scan delay.

A.3 Software Used

Origin, Gatan Micrograph, Image J, CASA XPS, CHI660e and Chem Draw.

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