

Research Article

Biogenic Synthesis of High-Performance α -MoO₃ Nanoparticles from Tryptophan Derivatives for Antimicrobial Agents and Electrode Materials of Supercapacitors

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Molybdenum trioxide nanoparticles (MoO₃ NPs) are recognized for their applications in novel multifunctional devices. Here, a biogenic, environmentally friendly method using *Lepidagathis cristata* leaf extract was employed to synthesize MoO₃ NPs. The as-obtained MoO₃ NPs exhibited a predominant (0 k0) orientation, representing an α -MoO₃ structure. The absorption band at 984 cm⁻¹ observed in the Fourier-transform infrared spectrum corresponded to the terminal Mo=O bond, thereby confirming that the prepared MoO₃ NPs were in the orthorhombic phase. Scanning and transmission electron microscopy data revealed that the MoO₃ NPs were well crystallized and uniformly distributed with grain sizes in the 70-100 nm range. The biogenic MoO₃ NPs demonstrated an excellent zone of inhibition against the selected Gram -ve and Gram +ve bacterial strains, thus providing an alternative to standard antibacterial agents. During electrochemical experiments conducted in a 1 M aqueous Na₂SO₄ solution, cyclic voltammetry (CV) curves of the MoO₃ NPs showed a pseudocapacitive nature, with a high discharge specific capacitance of 294 F/g and good cyclability. These results suggest the feasibility of the proposed biogenic, environmentally friendly method for preparing MoO₃ NPs for application in multifunctional devices.

1. Introduction

To minimize environmental pollution, plant-based green synthesis is being increasingly used for preparing metal oxide nanoparticles (NPs) for multifunctional applications [1–3]. Many physical and chemical methods are currently available for the synthesis of metal-oxide NPs. Physical techniques typically involve evaporation and condensation; thus, they are expensive due to the high energy required to maintain the high pressure and temperatures and the need to use highly sophisticated equipment. Chemical methods use chemical reductants such as ethanol, ethylene glycol, and

NaBH₄. However, these methods have the drawbacks of generating hazardous by-products and environmental contaminants and the use of expensive chemicals. Furthermore, chemical synthesis can lead to the binding of toxic chemical species to the surfaces of the produced NPs, which can negatively impact the environment [4, 5]. Hence, alternative methods are being developed for the synthesis of NPs using plant materials [6, 7]. Compared to physical and chemical methods, biogenic synthesis is advantageous as it uses less expensive resources and nontoxic materials only; moreover, it can achieve a high yield of NPs [8]. In particular, the biogenic synthesis of metal oxide NPs can yield NPs suitable for

dual applications. Recently, Pongam seed shells were used for synthesizing a carbon cobalt oxide porous composite, which was suitable for use in nonenzymatic glucose sensors and supercapacitor electrodes [9]. Cu-doped TiO_2 NPs were synthesized from *Cedrus deodara* extract, and the obtained nanoparticle was applied for dye degradation and antibacterial applications [10]. *Mimosa pudica* leaf extract was used for the synthesis of CuFeS_2 NPs, and the obtained NPs were used as electrodes for supercapacitors and for the photodegradation of methylene blue under solar irradiation [11]. Biogenic MoO_3 microrods were synthesized using *Azadirachta indica* leaf extract for cationic dye degradation and antibacterial applications [12]. Morphology-dependent CuO nanoparticles were synthesized via a green synthesis approach; the obtained nanoparticles had high size and surface area, and they showed good absorption efficiencies for the removal of harmful dyes and good antibacterial activity [13]. In the above studies, biogenic molecules were used for the synthesis of different NPs, and their properties were characterized after use in multifunctional applications in different domains. In this study, we prepared molybdenum trioxide (MoO_3) NPs for dual application using a biogenic synthesis.

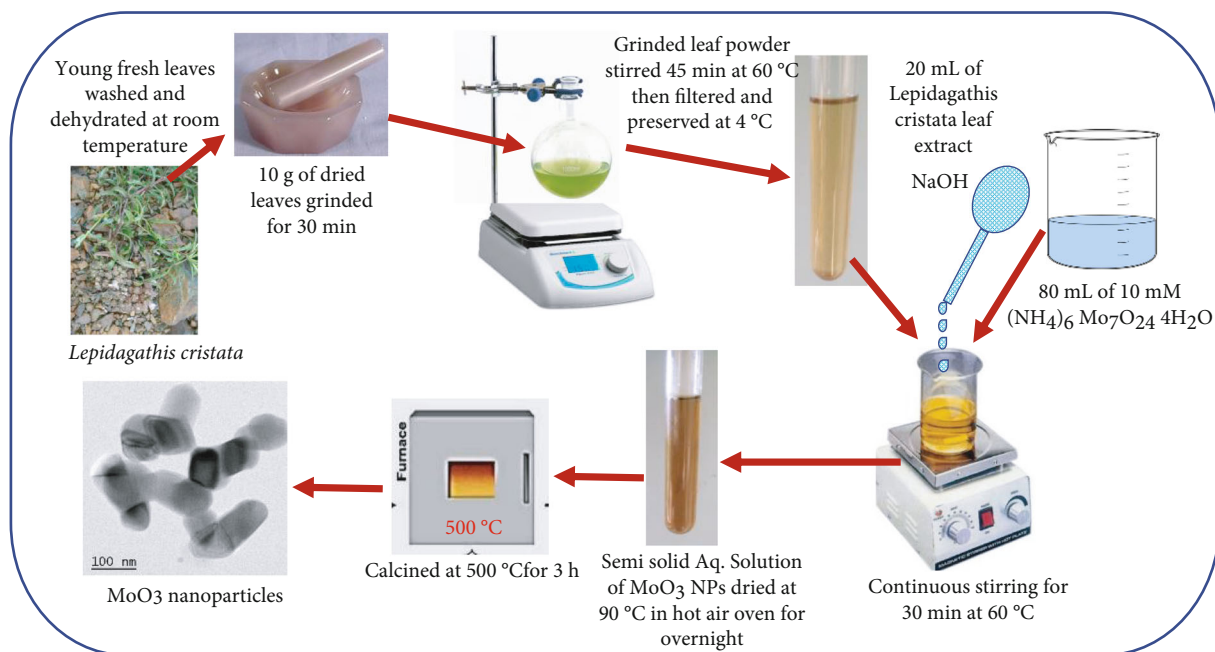
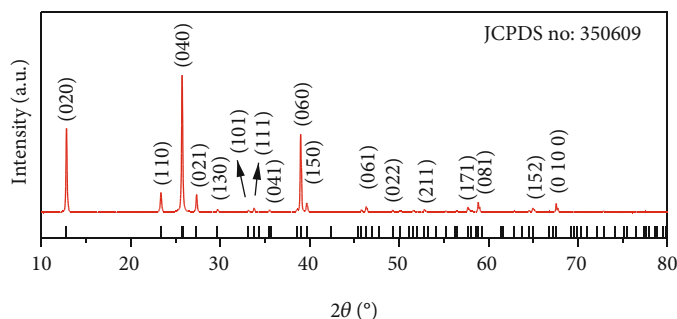
Among various metal oxide NPs, MoO_3 NPs are an appealing class of layered transition metal oxides. They have a variety of valence states and crystal structures in stable and metastable states. MoO_3 NPs exhibit three polymorphs, namely, orthorhombic (α - MoO_3), hexagonal (h- MoO_3), and monoclinic (β - MoO_3) structures. Over the past decade, researchers have focused on the synthesis of MoO_3 nanostructures with novel properties for multifunctional device applications. MoO_3 NPs and their composites have been used as gas sensors [14] and as electrode materials for energy conversion and storage [15, 16]. They have been effectively used in various catalytic reactions such as alcohol oxidation [17], epoxide ring-opening [18], ethanol oxidation, oxygen reduction [19], n-dodecane oxidation [20], sulfide to sulfate oxidation [21], and olefin epoxidation [22]. Moreover, MoO_3 NPs are multifunctional due to their unique layered structures and the wide range of oxidation states of different polymorphs. These multifunctional properties depend on the synthesis method, particle size, and shape. Thus, considerable efforts have been directed toward MoO_3 NP synthesis. For example, MoO_3 NPs were prepared via a hydrothermal method, and the obtained hexagonal NPs showed antimicrobial, antioxidant, and cytotoxic effects for the degradation of ketamine [23]. An α - MnO_2 /h- MoO_3 nanocomposite was synthesized via a chemical precipitation method and tested for supercapacitor electrode and photocatalytic activities [24]. h- MoO_3 nanorods were developed via a coprecipitation route and used for antimicrobial applications and to examine cytotoxicity against lung and breast cancer cells [25]. h- MoO_3 NPs were prepared via a hydrothermal method, and they demonstrated good photochromic and electrochromic properties [26]. α - MoO_3 NPs were prepared via a solution combustion method, and their photocatalytic and electrochemical properties were examined [27]. In another study, MoO_3 NPs were synthesized via a chemical precipitation method, and their optoelectrochemical properties, biocompatibility, and bioimaging were investigated [28]. The photocatalytic, glucose sensing,

and supercapacitor characteristics of nickel molybdate NPs were investigated using the molten salts technique [29]. The above studies synthesized and characterized MoO_3 and its composite nanostructures as multifunctional materials for different applications. However, the abovementioned conventional chemical methods are not environmentally friendly; alternative methods involving nanomaterial production via green synthesis and biogenic molecules extracted from plant sources are more environmentally friendly and less expensive compared to the physical and chemical methods.

Since different metals like copper, silver, gold, and other metals have been used in medicine frequently since antiquity and because these metal NPs have an antimicrobial nature, researchers have been interested in producing various metals, metal oxides, and metal composites that are resistant to microorganisms [30]. Present global demands fulfill to develop the novel NPs as alternative for traditional antimicrobial resistant agents. In general, NPs having high surface to volume ratio (S/V) than the precursor can vigorously interact with the cell membrane of the microorganism [31]. Mainly, NPs were vigorously interacting with sulfur and phosphorus of the biomolecules or genetic material and destroy the internal metabolic process (mainly replication), leading it to microorganism death [32]. Additionally, these NPs were synthesized using biogenic green techniques, which are crucial to preventing environmental damage. Hence, the use of plant crude extracts has advantages over other green technology procedures because plant crude extracts can minimize reaction times and maintain cell cultures [33, 34]. Plant extracts contain various active biomolecules that are actively involved in NP synthesis and inhibit particle agglomeration. They have also been used to synthesize NPs from *Bacillus pasteurii* [35], *Hydrangea paniculata* [36], *Camellia sinensis* [37], *Prunus persica* [38], and *Calotropis gigantea* [39]. To the best of our knowledge, no studies have reported biogenically synthesized α - MoO_3 NPs utilizing *Lepidagathis cristata* aqueous leaf extract for antibacterial and supercapacitor applications. In this study, nanocrystalline α - MoO_3 NPs were synthesized via an economically viable and environmentally friendly biogenic method using *L. cristata* leaf extract. Thereafter, the antibacterial activity of the biogenically synthesized α - MoO_3 NPs against Gram +ve and Gram -ve bacteria was demonstrated. The prepared MoO_3 electrodes also exhibited enhanced specific capacitance.

2. Material and Methods

2.1. Preparation of MoO_3 NPs. For the synthesis of MoO_3 NPs, aqueous leaf extract (20 mL) was mixed with ammonium heptamolybdate tetrahydrate (80 mL, 10 mM (0.98 g) of $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}\cdot 4\text{H}_2\text{O}$) solution in a 250 mL beaker and shaken well. Sodium hydroxide was added dropwise to the reaction mixture to maintain a neutral pH at 60°C for 30 min on a magnetic stirrer. The reaction mixture was heated in a hot air oven at 90°C overnight. The resultant semisolid was placed in a muffle furnace and calcined at 500°C for 3 h to produce MoO_3 NP powder [40, 41]; this was stored in a moisture-free environment for future use

SCHEME 1: Illustration of the synthesis procedure of MoO₃ NPs.FIGURE 1: XRD pattern of synthesized MoO₃ NPs.

(Scheme 1). The yield of the final obtained product is about ~0.9 g.

The details of the collection of plant crude extract, processing, and characterization of the samples are provided in the supporting information.

3. Results and Discussion

3.1. Microstructural Analysis. The X-ray diffraction (XRD) spectrum of the synthesized MoO₃ NPs is shown in Figure 1. The predominant peaks at 12.7°, 25.6°, and 38.9° correspond to the (020), (040), and (060) reflections of MoO₃, respectively. The identified sharp peaks are a manifestation of the highly anisotropic α-MoO₃ phase and the crystalline nature of the MoO₃ NPs [42]. The obtained XRD pattern, not only matched predominant peaks but also well matched with the minor peaks at 33.1° and 33.7° belonging to the (101) and (111) planes, respectively. The obtained lattice parameters were $a = 3.963 \text{ Å}$, $b = 13.856 \text{ Å}$, and $c = 3.969 \text{ Å}$, demonstrating that the synthesized MoO₃ NPs had an orthorhombic structure with the P_{bnm} space

group (good agreement with JCPDS card no. 350609). The Scherrer equation was used to calculate the average crystallite size of the MoO₃ NPs based on the predominant peaks.

$$D_p = \frac{0.94\lambda}{\beta \cos\theta}, \quad (1)$$

where λ is the X-ray wavelength (1.5406 Å), β is the full width at half maxima (FWHM) of the corresponding peak, and θ is the diffraction angle of the orientation. The calculated average crystallite size (D_p) of the MoO₃ NPs was 70 nm. The spectrum of MoO₃ NPs acquired using Fourier-transform infrared spectroscopy (FTIR) in the 400–4000 cm^{-1} wavenumber range is shown in Figure 2. The major characteristic absorption peaks were observed at approximately 453, 578, 806, 856, and 984 cm^{-1} . The absorption band at 984 cm^{-1} was attributed to the terminal M=O bond confirming that the MoO₃ NPs were in the orthorhombic α-MoO₃ phase [43]. The bridging of the intermediate oxygen atoms in the O–Mo–O bond was related to the absorption stretching frequencies at 806 and 856 cm^{-1} .

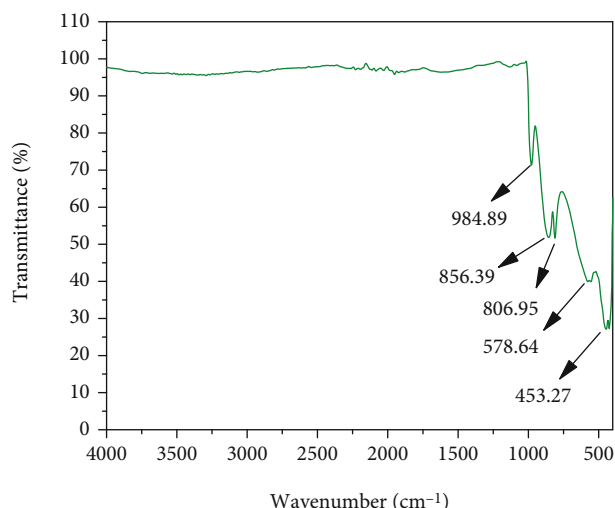


FIGURE 2: FT-IR spectrum of the synthesized MoO₃ NPs.

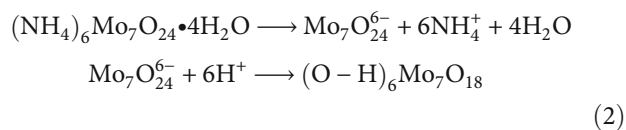
The bending mode of the Mo–O–Mo unit triggered the peak at 578 cm⁻¹, indicating that the molybdenum atoms shared an oxygen atom. The deformation vibrational modes were responsible for the absorption band at 453 cm⁻¹ [44]. The assignment of the observed frequencies is well supported by the XRD data.

X-ray photoelectron spectroscopy analysis of the prepared MoO₃ NPs was carried out, and the obtained survey spectra are shown in Figure 3(a). The presence of Mo, O, and C is in a highly pure state. The obtained peak at ~284.8 eV corresponds to the carbon (C) element. The C is the material which is always present in the atmosphere, so a nanolevel layer is deposited on every type of sample. Since XPS is surface sensitive, it practically always has a presence of carbon peak. The other peaks belong to Mo 3d, Mo 3p, Mo 4p, O 1s, and O KLL. Mainly, Mo3d and O1s peaks are observed at binding energies of ~232.5, ~235.6, and ~530.4 eV. Figure 3(b) shows the deconvoluted peaks of Mo3d_{3/2} and Mo3d_{5/2}, corresponding to the Mo⁶⁺ oxidation state of Mo [45]. The Mo 3d region showed a good separation of ~3.15 eV between two spin-orbit components. Figure 3(c) shows the O1s spectra of MoO₃ NPs. The spectra were deconvoluted into the O1, O2, and O3 peaks corresponding to the metal oxide, lattice oxygen, and defect O in the material, respectively [46]. The surface morphology of MoO₃ NPs is shown in Figure 4(a); the particles were well dispersed and had an estimated average grain size of approximately 100 nm. The energy-dispersive X-ray spectroscopy spectrum (Figure 4(b)) displayed Mo and O elements at their respective binding energies, and no other elements were observed, thereby indicating the purity of the obtained MoO₃ NPs. Figure 5(a) shows a transmission electron microscopy (TEM) image of the MoO₃ NPs. The NPs were spherical, and their sizes were in the range 50–70 nm. Figure 5(b) depicts the high-resolution TEM (HR-TEM) images, and the identified fringe width is 0.344 nm, which is well matched with the (040) diffraction plane in the standard data. Figure 5(c) shows the selected area electron diffraction (SAED) pattern of the MoO₃ NPs; sharp diffraction spots are observed with blurred rings, indicating that the particles were in the nanometer

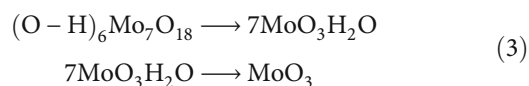
range. The identified fringes of (040), (141), (130), and (131) were well matched with the MoO₃ diffraction planes (JCPDS card no. 350609).

The zeta potential and particle size distribution data are shown in Figures S1a and S1b, respectively. The zeta potential of the MoO₃ NPs was estimated to be -34.6 mV. This elevated negative value indicated that the NPs were stable for a long time. At a scattering angle of 90° and wavelength of 530 nm, the estimated average particle size was 82 nm, and the polydispersity index value was 1.360. The active biomolecules in young *L. cristata* leaf extracts were effectively involved in the NP synthesis. Figure S2 shows the UV-Vis absorption spectra of *L. cristata* and the prepared MoO₃ NPs before and after the calcination. The results revealed that the MoO₃ NPs showed maximum absorption at approximately 250 nm (UV-C and UV-B regions), which may be attributed to the ligand-to-metal charge transfer (Mo–O), whereas the leaf extract did not show any UV-Vis absorption. Figure S3 shows the results of the N₂ adsorption and desorption measurements used for the evaluation of the specific surface area of the MoO₃ NPs. The obtained curve showed the type-IV isotherms, and the specific surface area is 3.648 m² g⁻¹.

Molecular self-assembly is an important phenomenon and a potential strategy for constructing an ensemble of nanostructures. Numerous plants include a variety of biologically active substances that function as reducing agents for metal salts, including alkaloids, phenols, flavonoids, ascorbic acid, citric acid, polyphenols, terpenes, and reductase. These biogenic molecules are effectively involved in the synthesis process; therefore, this process is generally applicable to the synthesis of several metal oxide NPs [47, 48]. Ravikanth et al. [49] extracted *L. cristata* leaf extract that contains mainly tryptophan derivative alkaloids; these alkaloids were actively involved in the synthesis of NPs. In this study, we used *L. cristata* leaf extract to synthesize MoO₃ NPs. The main content of this leaf extract is tryptophan derivative alkaloid, which was effectively involved in the synthesis process to obtain MoO₃ NPs [49]. The tryptophan derivative alkaloid did not induce any environmental toxicity in the formation of MoO₃ NPs. Chiang and Yeh [50] effectively prepared MoO₃ NPs by the reduction of ammonium heptamolybdate tetrahydrate using ethylene glycol, where the main role of ethylene glycol and tryptophan derivative alkaloids was to release H⁺ ions and act as reducing agents. Alkaloids progressively act as reducing agent by transferring the H⁺ ions into the medium as it reacts with molybdate (Mo₇O₂₄⁶⁻) to produce MoO₃ NPs. This process is described as follows:



(H⁺ from tryptophan derivative alkaloids.)



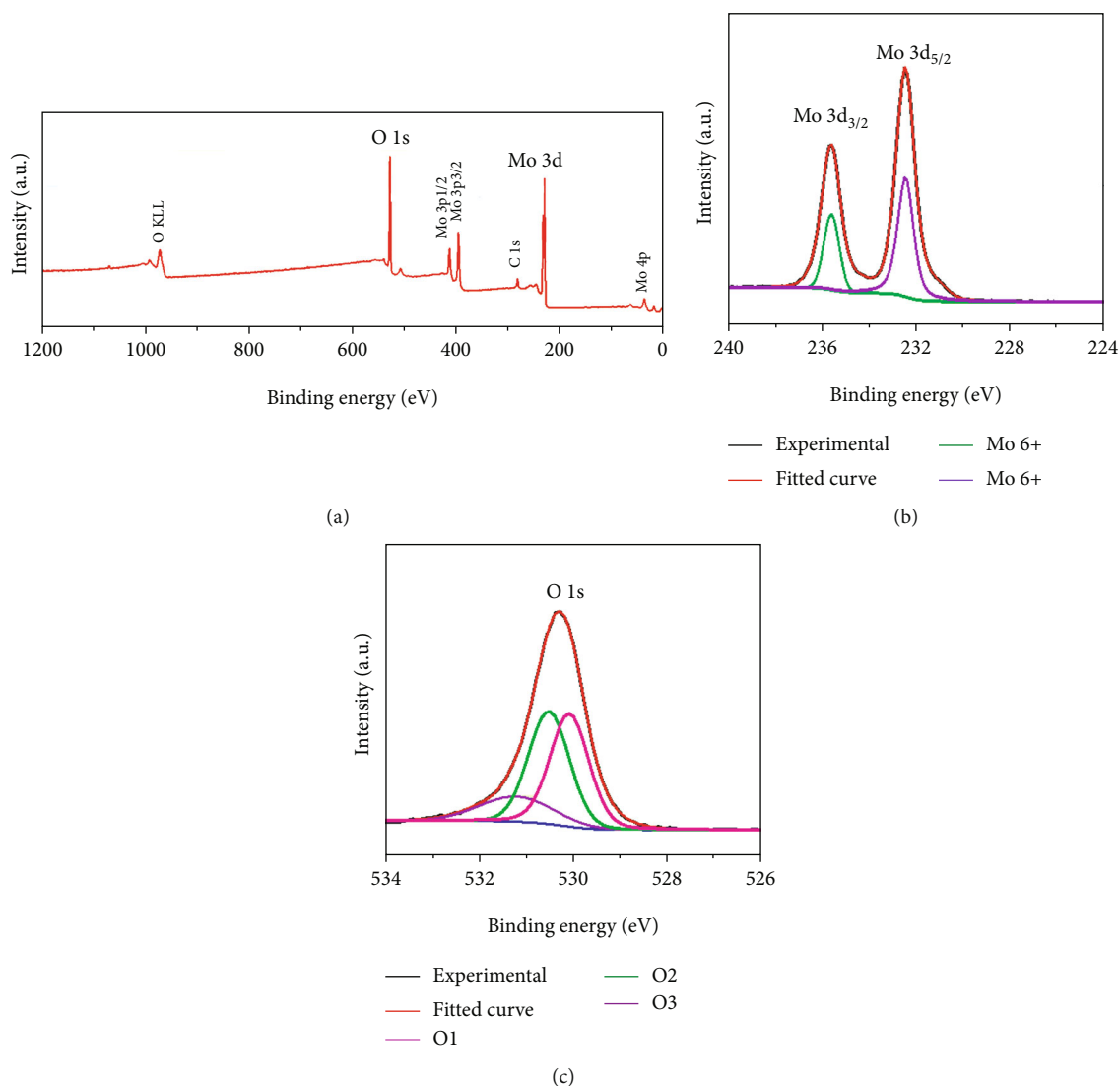


FIGURE 3: (a) Survey spectra of the synthesized MoO₃ NPs, (b) Mo3d core level binding energy spectra, and (c) O1s core level binding energy spectra.

The most probable reduction mechanism of MoO₃ occurred via the tryptophan derivative alkaloid (Figure 6). The tryptophan derivative alkaloid contains a diamond ring. The amide group resonates with the carbonyl group to form an imine functional group (structure (4)). The two structures are in equilibrium, and they shifted toward the imine ring because structure (4) was more stable than structure (1). The imine group was conjugated with the aromatic indole group; the stabilized structure extracted a proton from the nitrogen and attains more stability. Upon heat treatment, structure (5) of Mo₇O₂₄⁶⁻ was reduced to MoO₃ NPs. In this study, ammonium heptamolybdate tetrahydrate ((NH₄)₆Mo₇O₂₄·4H₂O) was successfully reduced by *L. cristata* leaf extract alkaloids, and it progressively acted as a reducing and capping agent. The obtained biogenically synthesized MoO₃ particles were further studied for their antibacterial activity and supercapacitive properties.

3.2. Antibacterial Activity. Metal oxide NPs are positively (+ve) charged, whereas microorganisms are negatively

(-ve) charged. These opposite charges give rise to electrostatic interactions between the microorganisms and the metal oxide NPs, leading to the oxidation and control of the microorganisms. The NPs effectively attach to the cell walls and plasma layers of microorganisms and increase the permeability of the cell wall, breaking the plasma layers and destroying the internal components of the cell, ultimately leading to cell death [50, 51]. The microlevel MoO₃ NPs have higher surface areas that effectively interact with the cell surface of microorganisms and ultimately show better antimicrobial properties than macrolevel NPs. The antibacterial activity of MoO₃ NPs was investigated using the agar well diffusion method against pathogenic bacteria such as *Pseudomonas aeruginosa*, *Klebsiella pneumonia*, *Escherichia coli* (Gram -ve bacteria), and *Streptococcus aureus* (Gram +ve bacteria). Biogenic MoO₃ NPs (25 and 50 μL) were added to each well, and ampicillin (25 and 50 μL) was used as the standard. Figure 7 depicts the antibacterial activity and zone of inhibition of MoO₃ NPs, with the data

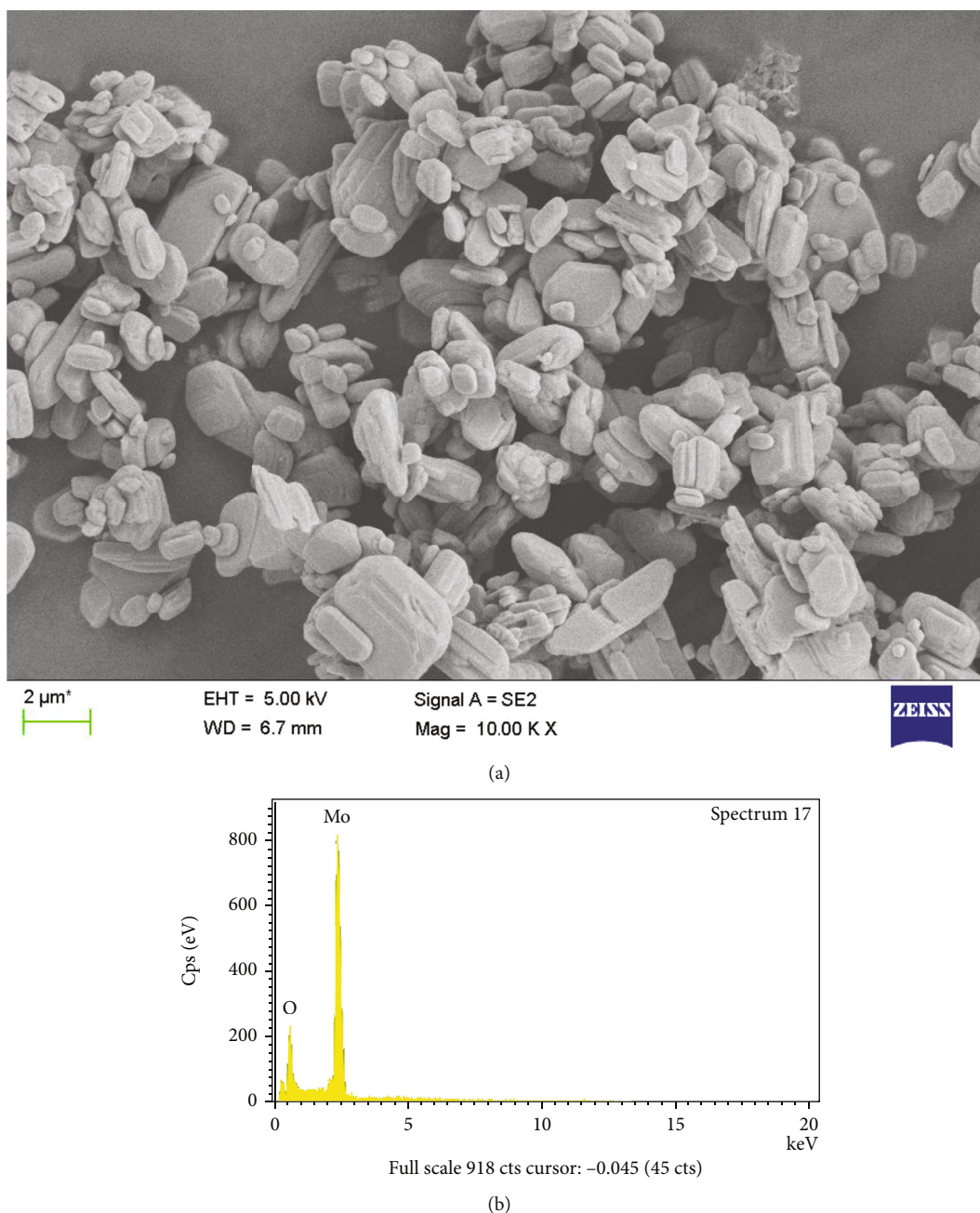


FIGURE 4: (a) SEM image and (b) EDS spectrum of the biogenically synthesized MoO_3 NPs.

summarized in Table 1. The Petri plates were incubated at 37°C for 24 hours and after incubation with proper precautions, the zone inhibition was measured in mm and the scale was inserted for effective comparison. Against the selected Gram -ve and Gram +ve bacterial strains, the biogenic MoO_3 NPs showed a good zone of inhibition. The Gram -ve bacteria exhibited a larger zone of inhibition than the Gram +ve bacteria. Generally, Gram +ve bacteria have very thick peptidoglycan cell walls, whereas Gram -ve bacteria have thin peptidoglycan cell walls and two cell membranes. The outer membrane of the Gram -ve bacteria affects the permeability of many molecules. Thus, MoO_3 NPs more

effectively interacted and rapidly entered the Gram -ve bacteria than the Gram +ve bacteria [23].

The zone of inhibition was examined for various concentrations of the MoO_3 NPs and ampicillin (standard). The maximum zone of inhibition was observed with $50\ \mu\text{L}$ of MoO_3 NPs and $50\ \mu\text{L}$ of standard ampicillin. MoO_3 NPs at $50\ \mu\text{L}$ concentration showed the maximum zone of inhibition against *K. pneumonia* (20 ± 0.7), whereas at the same concentration, it showed a small zone of inhibition against *S. aureus* (17 ± 0.3) and a moderate zone of inhibition against *E. coli* and *P. aeruginosa*. Furthermore, $50\ \mu\text{L}$ of ampicillin showed a good zone of inhibition against *E. coli*

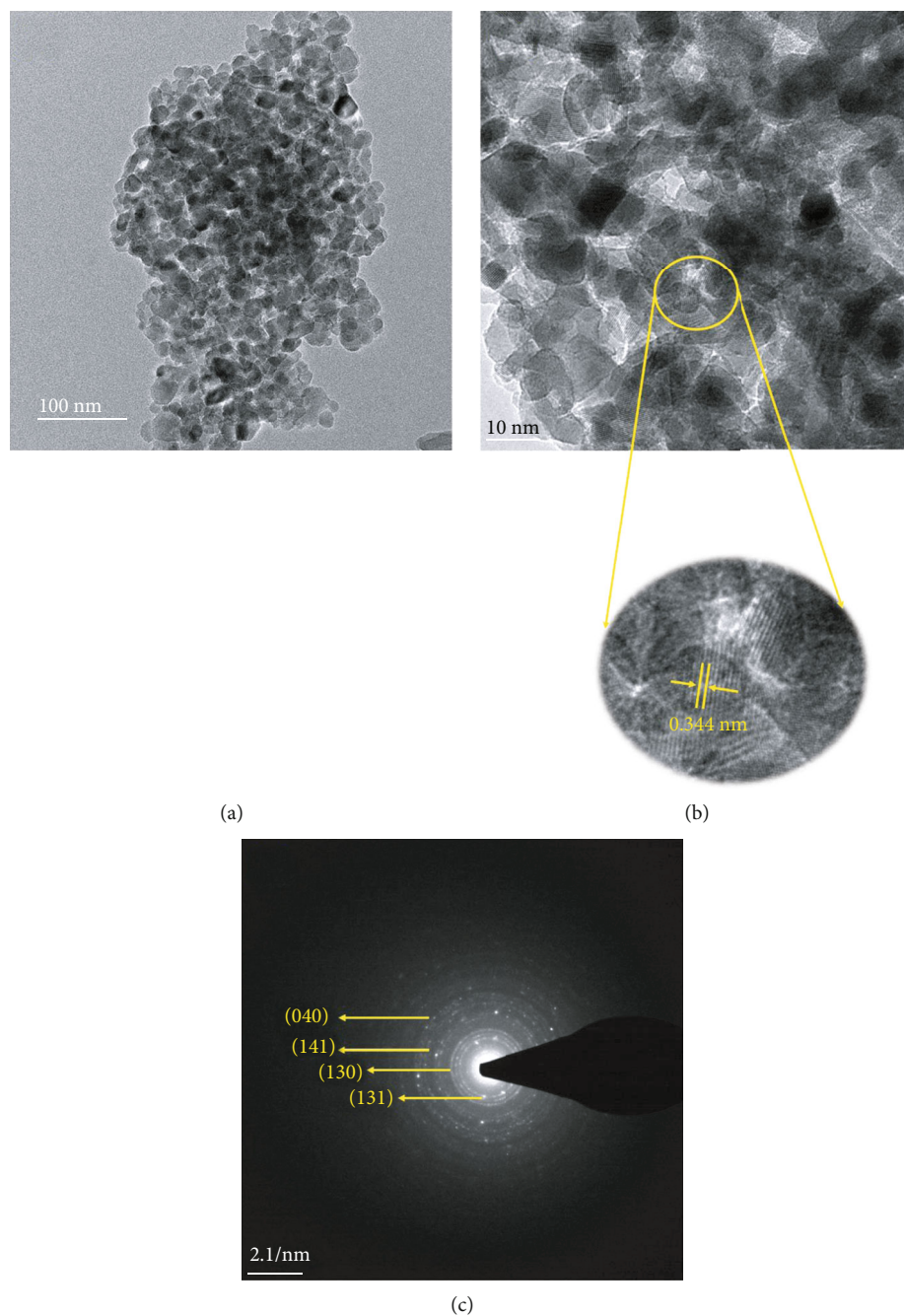
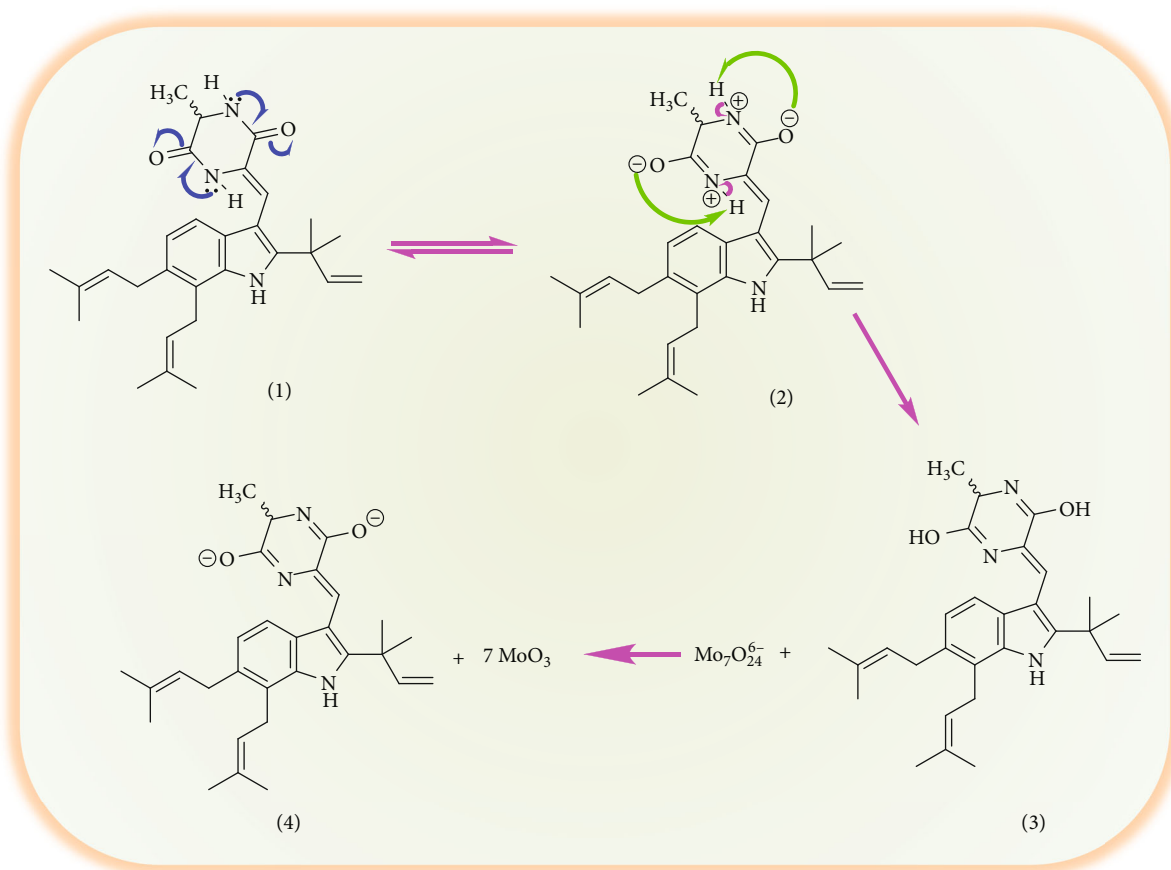
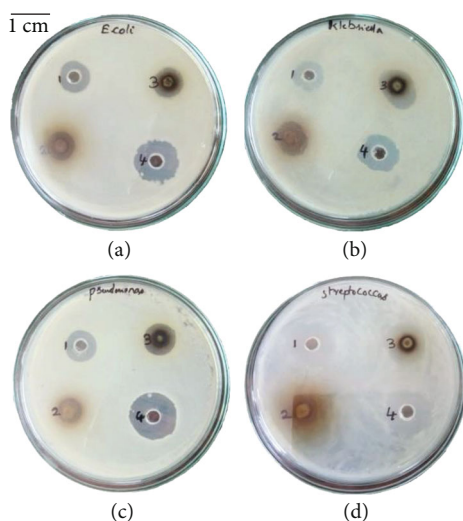


FIGURE 5: (a) TEM image, (b) HR-TEM images, and (c) SAED pattern of the synthesized MoO₃ NPs.

(22 ± 0.7) and *P. aeruginosa* (22 ± 0.5), whereas it showed a small zone of inhibition against *S. aureus* (20 ± 0.1). Fifty microliters of MoO₃ NPs showed a larger zone of inhibition against *K. pneumonia* than that obtained by the same concentration of ampicillin (standard). For better understanding, Figure 8 shows the bar graph for antibacterial activity and performed a one-way ANOVA (value of $p < 0.05$) test for statistical analysis using Microsoft Office Excel 2007; the results were considered significant.

Reports on the antimicrobial activity of MoO₃ NPs are scarce. MoO₃ NPs were prepared via electrochemical reduction and tested against *S. aureus* (Gram +ve) and *E. coli* (Gram -ve) bacteria. The zone of inhibition (in millimeters)

of *S. aureus* bacteria was 12.00 ± 2.00 , 15.66 ± 1.50 and *E. coli* bacteria was 10.66 ± 1.52 , 14.00 ± 1.00 for the 50 and 100 μL concentrations of the MoO₃ NPs, respectively [52]. MoO₃ nanorods were synthesized using a chemical bath deposition technique, and their antibacterial activities against *E. coli* (Gram -ve) and *S. aureus* (Gram +ve) were evaluated. The maximum zone of inhibition of the MoO₃ nanorods against Gram +ve bacteria was 3 mm whereas that against Gram -ve bacteria was 18 mm for ciprofloxacin standard drugs [53]. MoO₃ NPs were prepared via a hydrothermal method, and the observed zone of inhibition with 10 μL for Gram -ve bacteria (*E. coli*) was 13.41 ± 0.41 [23]. The enhanced performance of well-crystallized MoO₃ NPs

FIGURE 6: Reduction mechanism for the reduction of MoO_3 NPs.FIGURE 7: Zone of inhibition of bacteria: (a) *Escherichia coli*, (b) *Klebsiella pneumoniae*, (c) *Pseudomonas aeruginosa*, and (d) *Streptococcus aureus*.

synthesized in this study suggests that MoO_3 NPs provide an excellent alternative to the standard antibacterial agents. Moreover, the synthesis method was environmentally friendly and only used readily available natural sources.

3.3. Electrochemical Properties. The electrochemical properties of the MoO_3 NP electrode were tested using a three-electrode setup, in which the working, reference, and counter electrodes were MoO_3 NPs, Ag/AgCl , and platinum foil, respectively. The working electrode was prepared by mixing 80 wt.% MoO_3 NPs (active material), 15 wt.% carbon black (conducting agent), and 5 wt.% PVDF ($-(\text{C}_2\text{H}_2\text{F}_2)_n-$). These three were mixed with N-methyl-2-pyrrolidone ($\text{C}_5\text{H}_9\text{NO}$); the slurry was continuously stirred for 12 h, coated on a nickel (Ni) substrate, and dried at 100°C overnight. The average active mass of each electrode is ~ 0.0012 g [7, 8, 43]. First, we tested the variation of the current at different voltage scan rates (CV, cyclic voltammetry), performed chronopotentiometry (CP) at various current densities, and measured the impedance by electrochemical impedance spectroscopy (EIS) in a 1 M aqueous Na_2SO_4 electrolyte.

Figure 9 shows the CV curves of MoO_3 NPs in a potential range of 0.0–1.0 V recorded at different scan rates (1–100 mV/s). The asymmetric CV curves between the anodic and cathodic regimes indicated the pseudocapacitive nature of the MoO_3 NPs. The observed current values increased with increasing scan rate because the transfer rate of the Na^+ ions increased with the scan rate [24, 54, 55]. Equation (4) describes the Na^+ insertion process:

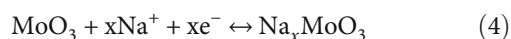


TABLE 1: Zone of inhibition (mm) of MoO₃ NPs against bacterial pathogens.

Type of the bacteria	Name of bacteria	Concentrations (μ L)			
		MoO ₃ NPs		Standard	
		25 μ L	50 μ L	25 μ L	50 μ L
		Zone of inhibition diameter $\pm$ SD (mm)			
		MoO ₃ NPs		Standard	
(Gram -ve)	<i>Escherichia coli</i>	15 $\pm$ 0.2	18 $\pm$ 0.6	15 $\pm$ 0.2	22 $\pm$ 0.7
	<i>Klebsiella pneumonia</i>	16 $\pm$ 0.6	20 $\pm$ 0.7	15 $\pm$ 0.6	20 $\pm$ 0.6
	<i>Pseudomonas aeruginosa</i>	14 $\pm$ 0.5	18 $\pm$ 0.3	15 $\pm$ 0.5	22 $\pm$ 0.5
(Gram +ve)	<i>Streptococcus aureus</i>	14 $\pm$ 0.2	17 $\pm$ 0.3	14 $\pm$ 0.5	20 $\pm$ 0.1

$\pm$ SD: standard deviation.

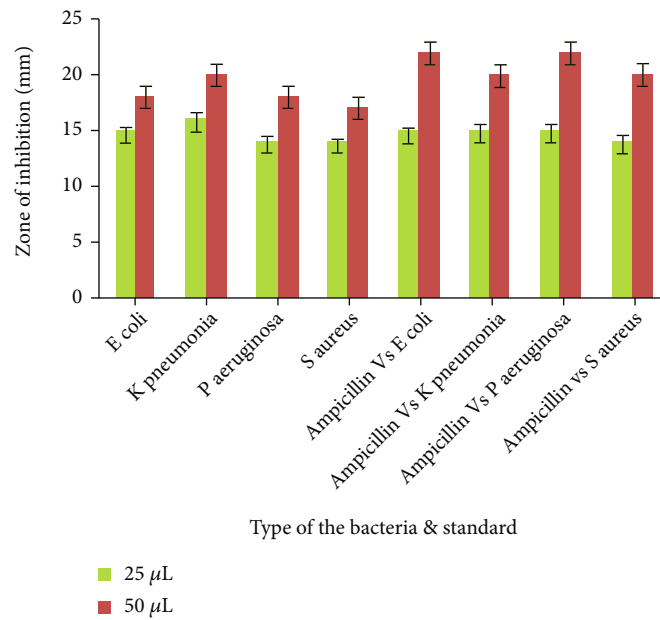
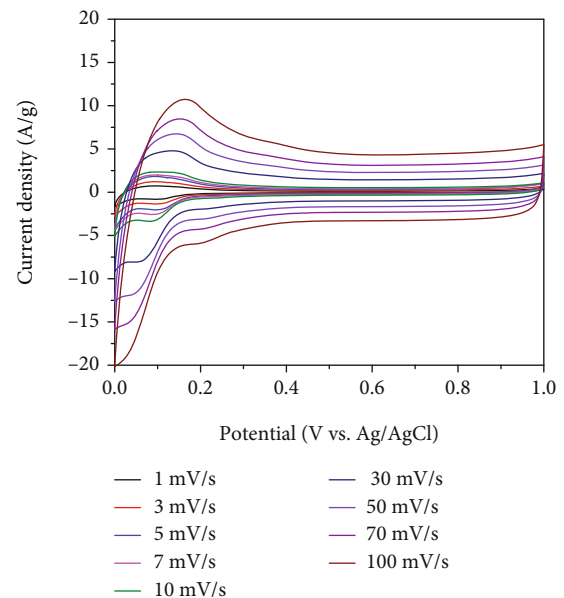


FIGURE 8: Statistical bar diagram of different bacteria.

CP measurements were conducted at different current densities to estimate the specific capacitance (C_s) of the MoO₃ NPs, as shown in Figure 9(a). The pseudocapacitive nature of the CP curves was confirmed by their nonlinearity, in agreement with the CV curves. The C_s of the electrode was determined using the CP curves and the following equation [56, 57]:

$$C_s = \frac{I\Delta t}{m\Delta V}, \quad (5)$$

where C_s denotes the specific capacitance (F/g), m denotes the active material's mass, ΔV (V) denotes the potential during discharge, I (A) denotes the average discharge current, and Δt denotes the total discharge time (s). At the current densities of 0.5, 1.0, 2.0, 3.0, and 5.0 A/g, the calculated C_s values of the prepared NPs were 294, 196, 157, 128, and 68 F/g, respectively. However, in Figure 10(a), because the Na⁺ ions were intercalated and deintercalated at a low current density of 0.5 A/g, most of the capacity has been acquired at a lower potential and fast discharge has been

FIGURE 9: CV curves of MoO₃ NPs at various scan rates.

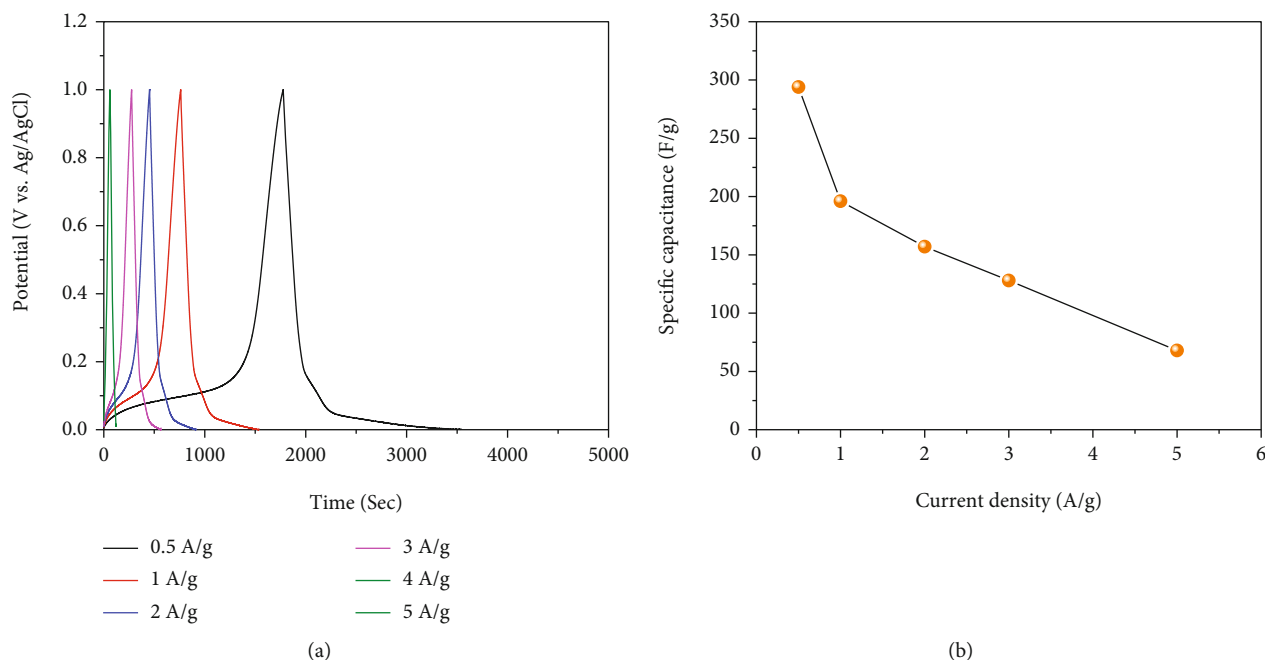


FIGURE 10: (a) CP curves of MoO₃ NPs at different current densities; (b) specific capacitance vs. current density of the MoO₃ NP electrode.

observed at a higher potential without IR drop. Figure 10(b) shows the specific capacitance (C_s) plotted versus the current density of the MoO₃ NP electrode. C_s increases monotonically at lower current densities because most of the cations (Na^+) intercalate on the surface and the inner active sites of the electrode [58]. The electrolyte ions had sufficient time to intercalate/deintercalate throughout the entire electrode material, and the oxidation/reduction peaks occurred at lower current densities, which is consistent with the CV traces [59].

Conducting EIS to determine the resistive and capacitive behavior of the electrode is crucial for determining the supercapacitor performance. Figure 11 shows the high-frequency (partial semicircle) and low-frequency (straight sloping line) zones in the Nyquist plot of the MoO₃ NP electrode for frequency between 1 Hz and 100 kHz. The data obtained before and after cycling were simulated using the ZSimpWin software and were fitted to the equivalent model circuit R(CR)(CR)W shown in the inset of Figure 10 (right upper side model circuit). The obtained solution resistance (R_s) and charge transfer resistance (R_{ct}) were $\sim 3.6 \Omega$ and $\sim 3.5 \Omega$, prior to long cycling, respectively, while the R_{ct} after 5000 cycles increased to $\sim 5.0 \Omega$, showing a marginal capacitance decrease across the long cycling process. This may be due to the occurrence of irreversible reactions involving the Na^+ electrolyte ions in the electrode material; such reactions increase the electrode resistance [58, 60, 61].

The MoO₃ electrode was tested using CP measurements over 5000 continuous cycles in a voltage ranging from 0.0 V to 1.0 V at a current density of 5 A/g. Figure 12 shows the C_s plotted vs. the number of cycles. Almost constant C_s up to 5000 discharge cycles was observed with 99% capacity retention. The inset shows the first and last five cycles of the elec-

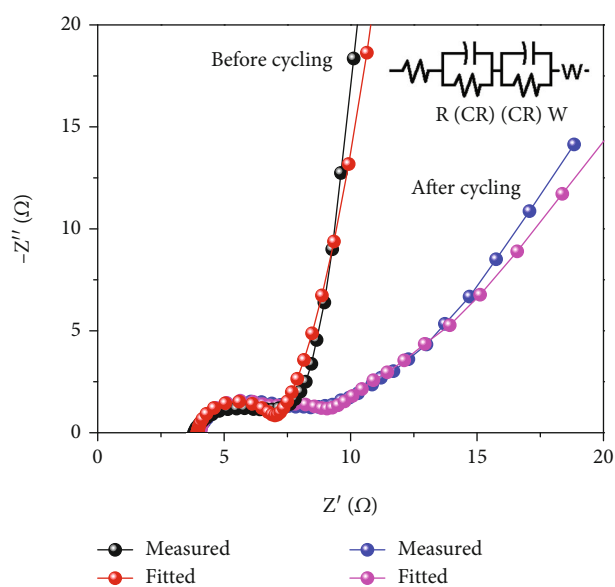


FIGURE 11: Nyquist plots before and after 5000 long cycles (inset: fitted graph).

trode during the long cycling process. Figures S4 and S5 show the XRD and SEM images of the electrode after long cycling process, and the observed XRD pattern and SEM image were like the before long cycling process, which represents the good stability of the MoO₃ electrode even after 5000 cycles at a current density of 5 A/g. To further improve the conductivity and rate performance of the MoO₃ NP electrode, carbonaceous or other suitable elements can be added or doped into the MoO₃. By acting as activators of the surface reactions and providing surface

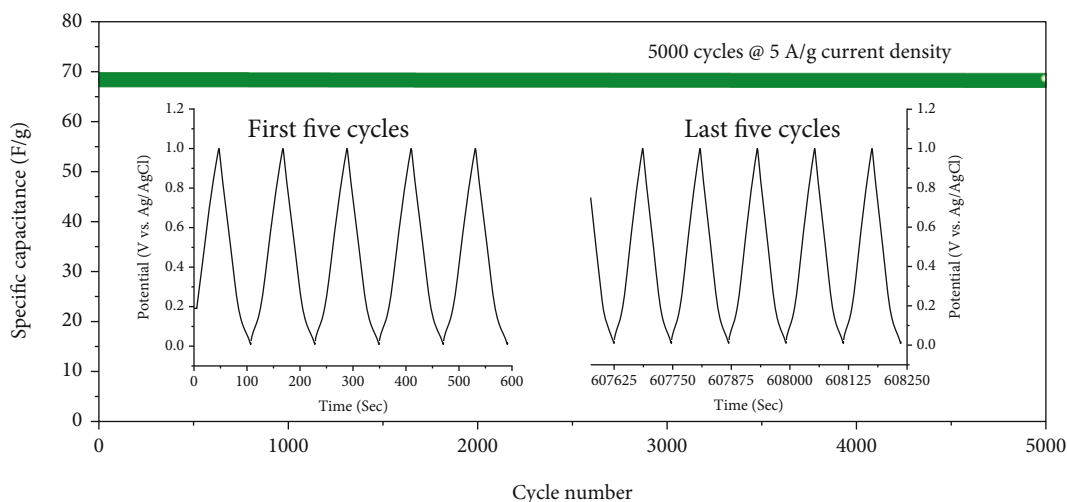


FIGURE 12: Cycling stability of MoO₃ NPs at a current density of 5 A/g. Inset shows first and last five cycles.

adsorption sites and electronic states, these additives can improve the electronic conductivity and rate performance of the MoO₃ NP electrode [62–64]. Recently, one-dimensional α -MoO₃ nanorods were prepared via a solution combustion method, and these achieved a C_s of 176 F/g for supercapacitor applications [65]. Silver NP-decorated MoO₃ prepared via a facile hydrothermal method exhibited a C_s of 225 F/g [66]. An MoO₃/PdO composite prepared by the sol-gel method using foliar fuel of *Euphorbia cognata* exhibited a capacitance of 127 F/g [67]. MoO₃ NPs modified with titanium dioxide NPs using the hydrothermal method attained a C_s of 141 F/g [68]. The use of bioactive *E. cognata* Boiss fuel for the sol-gel synthesis of MoO₃ NPs demonstrated a capacitance of 63.5 F/g [69]. A greener organic-inorganic framework functionalized MoO₃/ZnMoO₄ spherical electrode displayed a capacitance of 110 F/g [70]. The hydrothermally synthesized α -MoO₃ microspheres exhibited a capacitance of 201.4 F/g [71]. The hexagonal MoO₃ microrods were obtained via chemical bath deposition on stainless steel substrate, and their microstructural and electrochemical properties were studied for supercapacitor applications. From the electrochemical studies, the specific capacitance was obtained from CV curves as 194 F/g at 5 mV/s [72]. Additionally, catalase and enzyme-assisted chemical bath were used to deposit MoO₃ thin films for supercapacitor application, and specific capacitance of 560 F/g at a scan rate of 50 mV/s was obtained from the CV curves [73]. However, a biogenically synthesized MoO₃ NP electrode showed enhanced performance with a C_s of 294 F/g and was more competent than MoO₃ and its composite electrodes.

Moreover, an examination of the literature revealed that biogenically synthesized NPs exhibit multifunctional applications, such as antibacterial and supercapacitor applications. Recently, almond gum (*Prunus dulcis*) was used to synthesize ZnO NPs, and the obtained NPs exhibited antibacterial activity and supercapacitive properties [74]. Kimchi cabbage extract was used for the synthesis of Ag NPs, and the NPs were effective as antibacterial agents and as an elec-

trochemical supercapacitor electrode, exhibiting a C_s of 424 F/g [75]. *Aloe barbadensis* extract was used for the synthesis of nickel-doped copper ferrite NPs, and the obtained NPs showed enhanced antimicrobial activity against Gram +ve bacterial strains and a specific capacitance of 114 F/g as a supercapacitor electrode [76]. Gold, silver, and palladium NPs were synthesized from *Cissus quadrangularis* stem extract and deposited in an amorphous carbon matrix. The final product exhibited excellent antibacterial activity against Gram -ve bacteria and a maximum specific capacitance of 91 F/g as a supercapacitor electrode [77]. To the best of our knowledge, this is the first study to use *L. cristata* leaf extracts for the synthesis of MoO₃ NPs. The obtained MoO₃ NPs exhibited excellent antibacterial activity and, as a supercapacitor electrode, exhibited a maximum C_s of 294 F/g at a current density of 5 A/g with good cycling stability up to 5000 discharge cycles.

4. Conclusions

MoO₃ NPs were successfully synthesized via an environmentally friendly biogenic method using *L. cristata* leaf extract, and then, these were used for antibacterial and supercapacitor applications. The microstructure of the synthesized NPs was investigated, and it was observed that the NPs were in a stable orthorhombic phase with roughly spherical grains with a size of 70–100 nm. The estimated zeta potential of -34.6 mV indicated the good stability of the synthesized NPs. The biogenically synthesized MoO₃ NPs showed an excellent zone of inhibition for the selected Gram +ve and Gram -ve bacterial strains and thus can provide a suitable alternative to standard antibacterial agents. The supercapacitive behavior of the MoO₃ NP electrode material showed the highest C_s of 294 F/g at 0.5 A/g current density with good cyclability. In conclusion, the biogenically synthesized α -MoO₃ NPs are multifunctional materials that demonstrate good antibacterial activity and potential for use as electrodes for supercapacitors.

Data Availability

The data of the models or raw files that will be provided in this study are available from the corresponding authors by request.

Conflicts of Interest

The authors declare no conflict of interest in publishing this article.

Authors' Contributions

Nunna Guru Prakash and Siddarapu Himagirish Kumar contributed equally to this work.

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Supplementary Materials

Supplementary data includes the collection of plant crude extract and material characterization. Figure S1: (a) zeta potential and (b) particle size distribution of MoO_3 NPs. Figure S2: UV-visible absorption spectra of (a) *Lepidagathis cristata* leaf extract and (b) MoO_3 NPs before and (c) after calcination. Figure S3: N_2 adsorption-desorption isotherm of the MoO_3 NPs. Figure S4: XRD pattern of MoO_3 NP electrode after 5000 cycles. Figure S5: SEM image of the MoO_3 NP electrode of after 5000 cycles. (*Supplementary Materials*)

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