Synthesis of Conductive MOFs for Enhanced Electrochemical Performance as Anodes in Lithium-Ion Batteries

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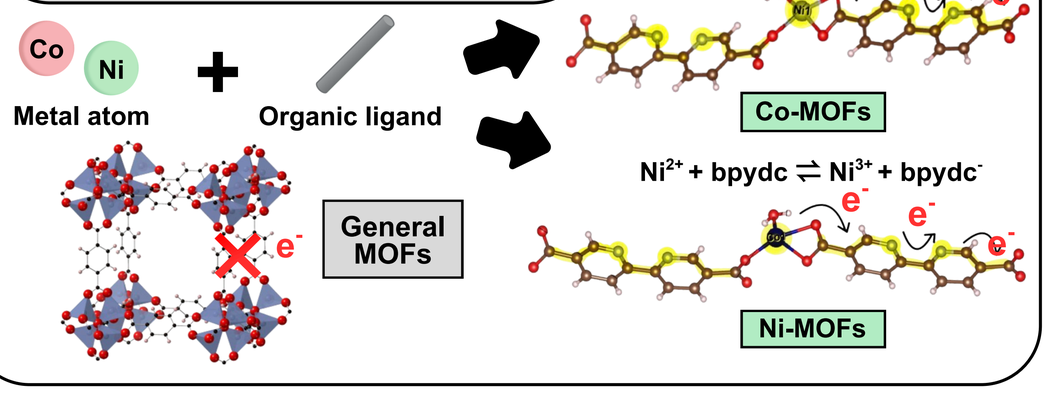
Abstract

Currently, Lithium-ion batteries (LIBs) have gained significant attention due to their high energy density, long cycle life, and excellent charge-discharge efficiency. However, commercial anode materials for LIBs still face limitations such as low electrical conductivity and restricted rate capability. This research focuses on the development of a novel anode material with enhanced structural and conductive properties by utilizing Conductive Metal–Organic Frameworks (C-MOFs). These materials possess a three-dimensional structure, high surface area, and the ability to conduct electricity through their metal-ligand frameworks. In this study, two transition metals, Cobalt (Co) and Nickel (Ni), were selected, along with the [2,2′-bipyridine]-5,5′-dicarboxylic acid (bpydc) ligand, to synthesize Co-bpydc and Ni-bpydc MOFs. Both metals are known for their electron transfer capabilities, which facilitate internal conductivity and are expected to enhance the potential of these materials as anodes for LIBs.

The research began with the synthesis of the organic ligand, which serves as the structural linker for the MOFs, via the reflux method at 106°C for 3 hours. The reaction progress was monitored using Thin-layer Chromatography (TLC) to ensure the complete consumption of precursors. The atomic structure of the synthesized ligand was verified using Nuclear Magnetic Resonance (NMR) spectroscopy, which showed peak positions consistent with reference data, confirming successful synthesis. Subsequently, the MOFs were synthesized using transition metals (Co, Ni, and Zn) through the hydrothermal method at 150°C for 48 hours to obtain the anode materials. Morphological characterization via light microscopy and Scanning Electron Microscopy (SEM) revealed that the synthesized Co-bpydc and Ni-bpydc exhibited micrometer-scale polygonal structures. Energy-Dispersive X-ray Spectroscopy (EDS) confirmed the elemental composition of the MOFs and the formation of coordination bonds between the metal ions and the ligands. Furthermore, crystal structure analysis was performed using Single Crystal X-ray Diffraction (SCXRD). Comparison with crystallographic databases indicated that both Co-bpydc and Ni-bpydc structures matched previously reported phases, confirming that the synthesized materials are known phases rather than novel structures.These synthesized materials will be utilized as anode materials in lithium-ion battery cells to evaluate their electrochemical properties and assess their potential for further practical applications.

Introduction

- **Problem :** The poor electrical conductivity of general MOFs limits their electrochemistry.
- **Solution :** Developing conductive MOFs.

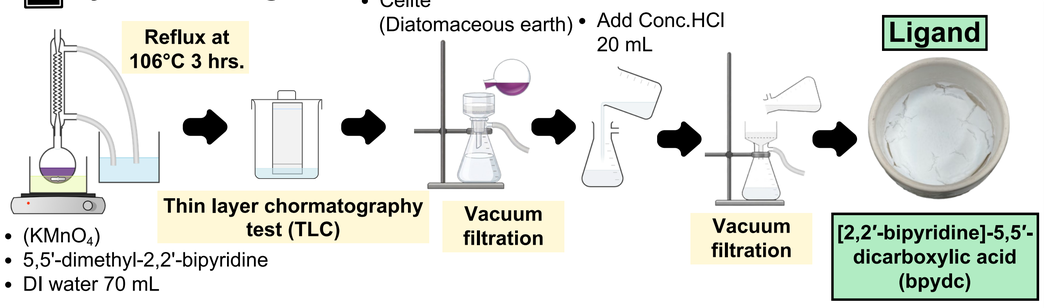


Objectives

1. To synthesize the ligand [2,2′-bipyridine]-5,5′-dicarboxylic acid (bpydc) as a precursor for the fabrication of conductive metal–organic frameworks.
2. To synthesize conductive metal–organic frameworks, namely Co-bpydc and Ni-bpydc, via a hydrothermal process.
3. To evaluate the electrochemical performance of conductive metal–organic frameworks, Co-bpydc and Ni-bpydc, as anode materials for lithium-ion batteries, including cycling stability, rate capability, cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS) analyses.

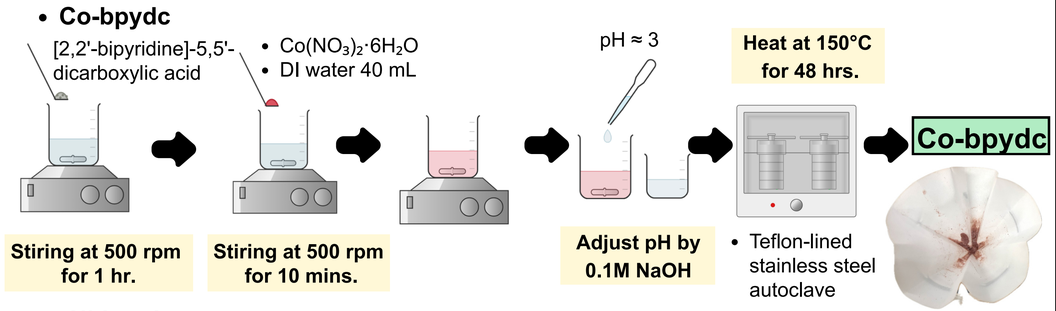
Experimental

1 Synthesis of ligand

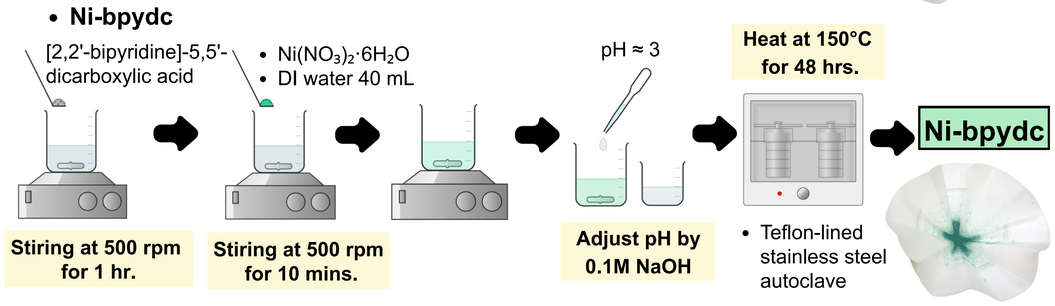


2 Synthesis of Co-bpydc/Ni-bpydc by hydrothermal method

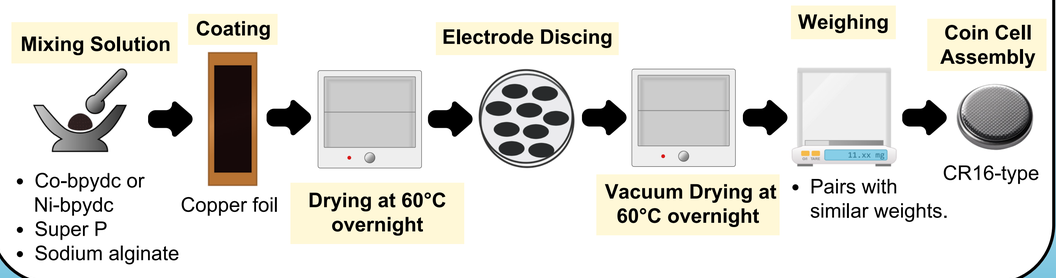
- **Co-bpydc**



- **Ni-bpydc**

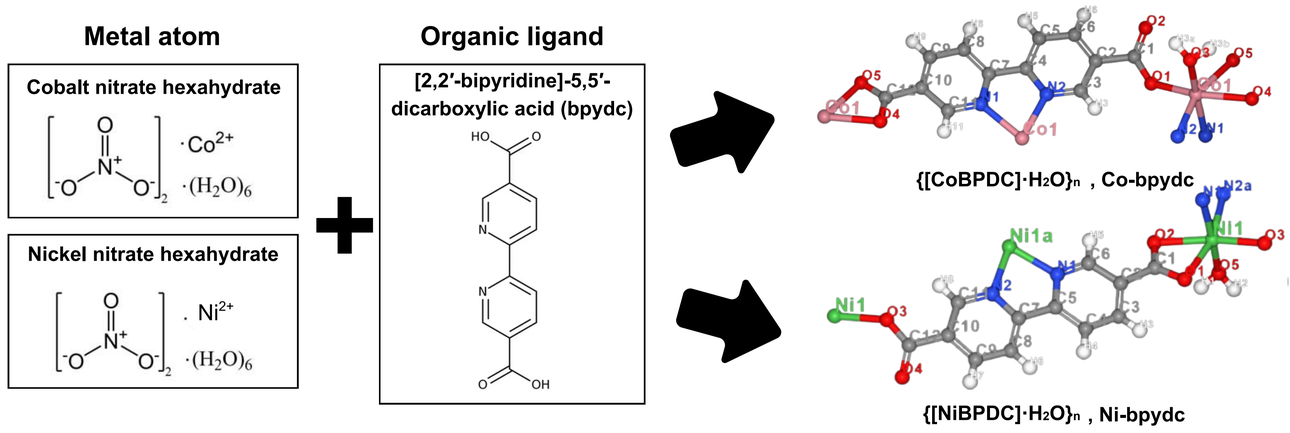


3 Synthesis of Co-bpydc/Ni-bpydc by hydrothermal method

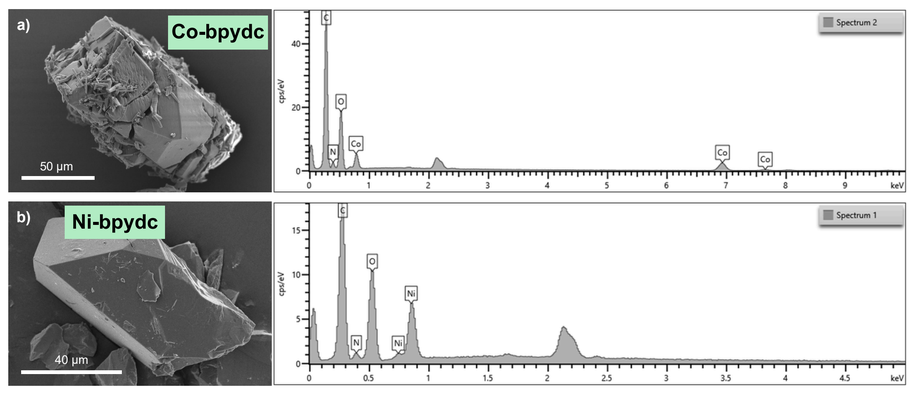


Results

• Single Crystal X-ray Diffraction (SCXRD) Result



• SEM and EDS



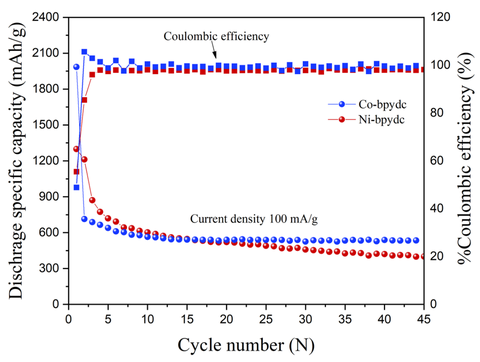
Element	Atomic %
N	9.64
Co	3.57

Element	Atomic %
N	7.01
Ni	8.06

- SEM image revealed a polygonal crystals for
- Co-bpydc and Columnar crystals for Ni-bpydc.
- EDS spectrum confirmed Co and Ni coordination with the ligand, verifying MOF formation.

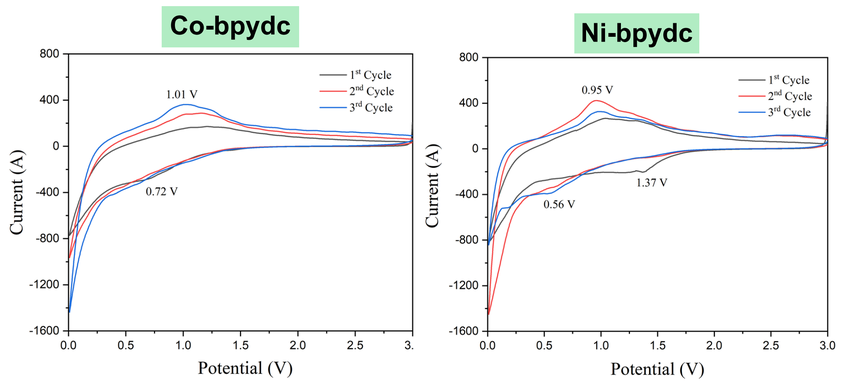
• Electrochemical Performance Evaluation

- **Cycling stability test**



- Cycling stability results show that Co-bpydc exhibits greater long-term stability than Ni-bpydc.

- **Cyclic voltammetry (CV)**



- Electrolyte + $Li^+ + e^- \rightarrow$ SEI (0.56 V, 0.72 V)
- $M^+ Li_2O \rightarrow M^{2+} + 2Li^+ + 2e^+$ (0.95 V, 1.01V)
- $M^{2+} + 2Li^+ + 2e^- \rightarrow M + Li_2O$ (1.37 V)

M = Co, Ni

Conclusions

- The NMR results confirmed the expected molecular structure of ligand [2,2′-bipyridine]-5,5′-dicarboxylic acid (bpydc).
- SEM and EDS confirmed the morphology and MOF formation, while SCXRD revealed the crystal structure of the MOF.
- Electrochemical tests demonstrate the effectiveness of the conductive MOF, with good cycling stability and high current response in cyclic voltammetry.

Acknowledgements

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