IIT MADRAS
Indian Institute of Technology Madras

Technology Transfer Office
TTO – IPM Cell

Industrial Consultancy & Sponsored Research (IC&SR)

PETACENETETRAONE (PT) AND ITS DITHIIN DERIVATIVE AS A CATHODE MATERIAL FOR ORGANIC AQUEOUS ZN-ION BATTERIES

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Problem Statement & Unmet Need

- Currently, aromatic quinones are used as promising **cathode materials for Zn-ion batteries, but they are plagued with low voltages in contrast to inorganic materials.**
- Hence, there is a need in the art to develop a **working electrode extensively for aqueous Zn-ion batteries with high capacities**

Technology Category/ Market

Category – Energy, Energy Storage & Renewable Energy /Advance Material & Manufacturing
Applications –Power Grids, Transport, Railway Power Supplies, Remote Controls and Flashlights
Industry –Power Generation, Transport/Automobiles
Market -The Global Zinc-Ion Battery Market Size is valued at 9.10 billion in 2022 and is predicted to reach **12.30 billion by the year 2031** at a **3.55% CAGR** during the forecast period for 2023-2031.

Key Features / Value Proposition

Technical perspective

- ***Pentacene-5,7,12,14-tetraone(PT)*** as a novel cathode material for aqueous Zn-ion batteries shows **excellent reversibility for Zn^{2+} insertion/de-insertion with a single potential plateau**
- The electrode material incorporated with **CMK-3** exhibits capacity of **220 $mAhg^{-1}$** with polarization of 80 mV, **cycling stability up to 2000 cycle and rate capability event at 20 Ag^{-1}**
- Further, the **voltage of the Zn-ion battery is tuned by the incorporation of sulfur atoms in the PT molecular framework.**

User perspective

- **Higher energy density Zn-ion batteries with durability.**

TRL (Technology Readiness Level)

TRL-4 Technology Validated in Lab

Research Lab

Prof. KOTHANDARAMAN RAMANUJAM
Dept. of Chemistry

Intellectual Property

- **IITM IDF Ref. 1945**
- **IN202041020063**

Technology

- ***An organic electrode cathode material comprising pentacene-5,7,12,14-tetraone (PT) and its dithiin derivative, dibenzo [b,i] thianthrene-5,7,12,14-tetraone (SPT) for an aqueous metal-ion battery with an aqueous electrolyte:***
- The said cathode material is **encapsulated in a mesoporous conductive additive** to increase the electronic conductivity and cycling stability of the electrode, the said the conductive additive is **CMK-3 carbon**
- **Further discloses, a preparation of electrode material for organic aqueous Zn-ion batteries, steps comprising:**

1. **Grinding a mixture containing PT or SPT, super P or CMK-3 carbon black, and PVDF in 55:35:10 (w/w/w) ratios**
2. **Adding N methylpyrrolidone (NMP) to the well ground mixture to obtain a slurry**
3. **Coating the slurry on a stainless steel foil (current collector)**
4. **Drying the electrode overnight in an air oven at 70°C**

- The aqueous metal-ion battery is **Zn-ion battery,** and the electrolyte is **$ZnSO_4$**
- The strong π-stacking provides **stability to PT through delocalization of π-electrons** under electrochemical cycling
- Presence of **sulfur atoms in the molecular skeleton (SPT)** reduces the **LUMO energy** of the molecule, which results in a high voltage of the cell is improved by **120 mV in comparison to PT**

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Images

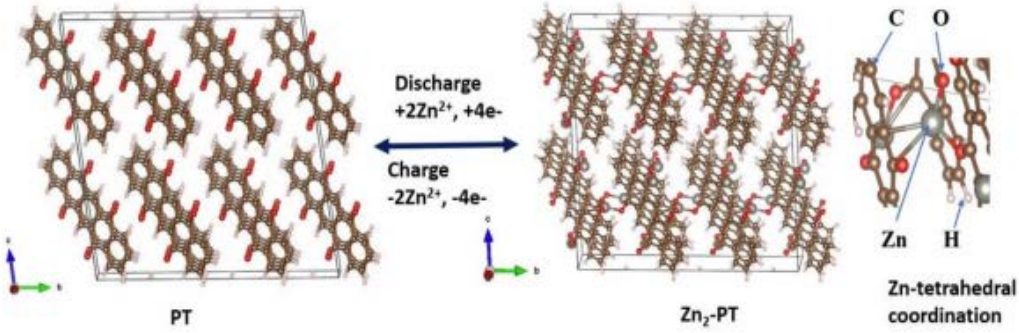

Figure 1 shows Zn^{2+} insertion mechanism of PT

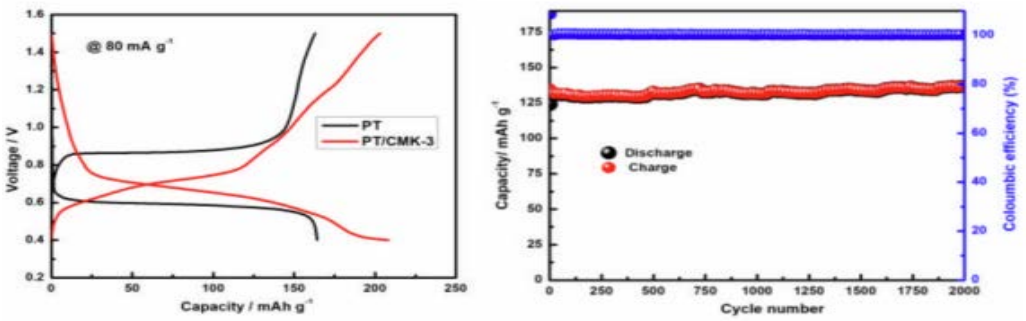

Figure 2 shows (a) comparison of discharge/charge voltage profiles of PT and PT/CMK-3 composite at a current density of 80 mA g-1 25 . (b) Cycling performance of PT/CMK-3 at a current density of 3 A

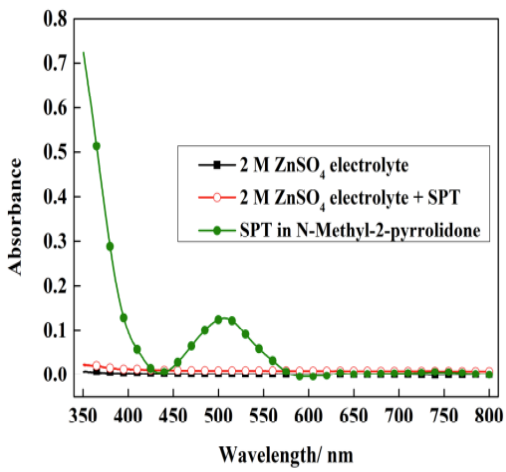

Figure 3 depicts UV-Vis spectra of **$ZnSO_4$** electrolyte, SPT dispersed **$ZnSO_4$** electrolyte and SPT dissolved N-methyl-2-pyrrolidone solution as reference.

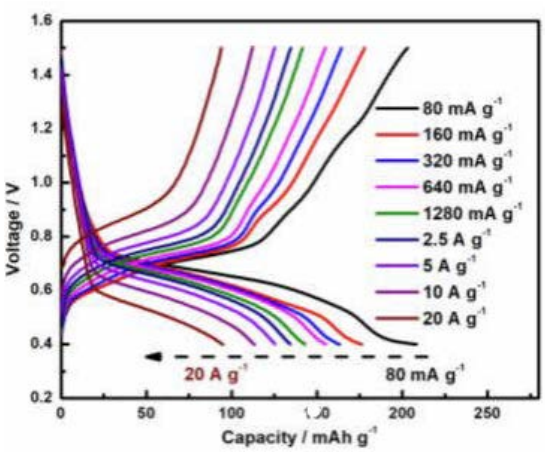

Figure 4 depicts rate capability of PT/CMK-3 at different current densities.

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