Electrochemical Characterization of Copper Phthalocyanine for Lithium-Based Batteries

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Abstract

Present an analytical formulation of the reversible voltage and electrode electrochemical kinetics at the interface between the active material, CuPc, and the electrolyte in a lithium-based cell.

Developed Theoretical Formulation

The reversible process of charge transfer at the CuPc – electrolyte interface under the external open – circuit condition is represented as:

\[ x \ g = \text{moles of Li}^+ \text{(in an electrolytic solution)} + x \ g = \text{moles of e}^- \text{(in an electronic conductor such as carbon)} + 1 \ g = \text{mole of host material, CuPc} \]

\[ \Rightarrow (x - g) = \text{moles of (Li}^+ \cdot \text{e}^- \text{) pairs in 1 g = moles of CuPc} \]

The equilibrium condition of electrochemical reaction process for a set of temperature and pressure conditions can be presented as:

\[ x \mu \text{chem} \text{(in electrolyte solution)} + x \mu \text{chem} \text{(in e}^- \text{conductor)} = x \mu \text{chem}( \text{in CuPc}) \]

Using the thermodynamic information, equation [1] is transformed to:

\[ E_{rev,T} = E_1^e + \left( \frac{RT}{F} \right) \ln \left( \frac{x \mu_{\text{Li}^+} \text{chem}}{x \mu_{\text{e}^-} \text{chem}} \right) - \ln \left( \frac{x \mu_{\text{Li}^+} \text{chem}}{F} \right) \]

Equation [2] shows the dependence of \( E_{rev,T} \) on the lithium ion concentration in the electrolyte in contact with the cathode electrode active site for the reversible process of charge transfer at the electrode.

\[ \Rightarrow i = \text{i eq} \left[ \frac{x \mu_{\text{Li}^+} \text{chem}}{R T} \exp \left( \frac{x \mu_{\text{Li}^+} \text{chem}}{R T} \right) - \exp \left( \frac{x \mu_{\text{Li}^+} \text{chem}}{RT} \right) \right] \]

Conclusions

a) Equation [2] shows the dependence of \( E_{rev,T} \) on the lithium content of CuPc and lithium ion concentration in the electrolyte in contact with the cathode electrode active site for the reversible process of charge transfer at the electrode.

b) The theoretical formulation, Eq. [8], shows the dependence of the total current on various parameters such as \( x, \ E, \ \alpha_a, \ \alpha_c, \ \text{etc.} \) at a given temperature.

c) Theoretical formulation can be employed in the design and performance analysis of a cathode electrode with the active material, CuPc.