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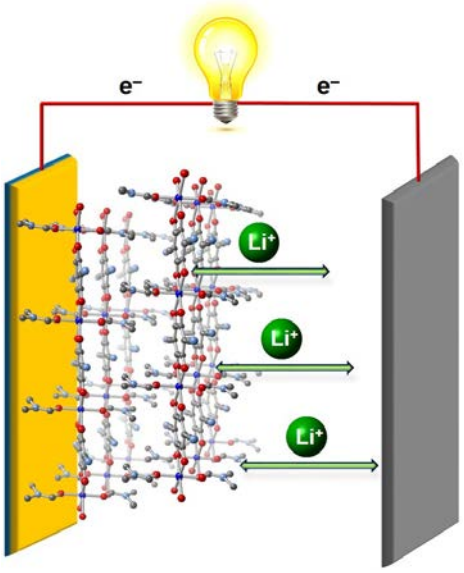
Elucidating metal and ligand redox activities of copper-benzoquinoid coordination polymers as high performance cathodes for lithium-ion batteries

Watchareeya Kaveevivitchai (柯碧蓮)[1,2*], Teng-Hao Chen (陳登豪)[3], Jeng-Lung Chen (陳政龍)[4]

[1]Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan
[2]Hierarchical Green-Energy Materials (Hi-GEM) Research Center, National Cheng Kung University, Tainan, Taiwan
[3]School of Pharmacy, National Cheng Kung University, Tainan, Taiwan
[4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan
wkaveechai@mail.ncku.edu.tw

Abstract

A novel redox-active quinone-based organic building block 1,4-dicyano-2,3,5,6-tetrahydroxybenzene (LH_4) has been synthesized and used as bridging ligand to form novel 1D copper-benzoquinoid coordination polymers $[CuL(DMF)_2]_n$ and $[CuL(Py)_2]_n$. The compound $[CuL(DMF)_2]_n$ is found to deliver an initial capacity as high as 268 mA h g^{-1} at 30 mA g^{-1} when used as cathode in lithium-based batteries. By replacing the axially-coordinated dimethylformamide (DMF) molecules on the Cu(II) in $[CuL(DMF)_2]_n$ with pyridine (Py) to yield $[CuL(Py)_2]_n$, the electrochemical performance is dramatically improved. Cu K-edge XANES and EXAFS measurements confirm the change in the oxidation state and coordination environment of Cu during the discharge–charge process. In combination with other characterization techniques, the synergistic effect of both Cu and organic moieties in the multi-electron redox reaction has been revealed. The fundamental understanding of the mechanism of these two compounds as electrode materials in lithium-ion batteries may pave the way for the design and development of other metal-organic compounds for the next-generation high performance energy storage systems.



Keywords – Metal-organic materials, Li-ion batteries, energy storage.

References

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