## **Exploration of Li-Organic Batteries Using Hexaphyrin as an Active Cathode Material**

Ji-Young Shin 1,\*, Zhongyue Zhang 2, Kunio Awaga 2 and Hiroshi Shinokubo 1

- <sup>1</sup> Department of Molecular and Macromolecular Chemistry, Graduate School of Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan; jyshinl@chembio.nagoya-u.ac.jp
- <sup>2</sup> Department of Chemistry, Graduate School of Science, Nagoya University
- \* Correspondence: jyshin@chembio.nagoya-u.ac.jp; Tel.: +81-52-747-6771



Figure S1. Cyclic voltammogram of Li-[28]hex batteries in 2~4.5 V range set.



**Figure S2.** Charge/discharge performances of Li-[28]hex battery: earlier (red) and later (blue) cycles: range = 2 ~ 4 V, number of cycles = 20, and operation current = 0.2 mA.



**Figure S3.** Potential energy diagram for the frontier molecular orbitals of Hückel antiaromatic and Möbius aromatic [28]hexaphyrins.



**Figure S4.** Battery performance Li-[28]hex battery over 1000 cycle: (a) charge/discharge performances (each  $10^{th}$  cycle was projected.), (b) selected charge/discharge graphs (C and D represent charge and discharge curves for the corresponding cycle, respectively.), and (c) capacity and efficiency plots for the 1000 cycle measurements: window's width = 2 ~ 3.8 V, operation current = 3 mA.



**Figure S5.** Background CV of pure carbon black for the Figure 3 within the voltage window of  $2.0 \sim 4.0$  V and a scan rate of 2.0 mV/s.



**Figure S6.** EIS plots before and after 200 cycles of charge/discharge performances. The significantly increased impedance suggests the formation of solid-state electrolyte interface (SEI) layers.