Electrochemical Performance of Truxenone and Related Condensed Fluorenones For Na-ion Battery

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Structurally flexible organic solids have been proposed to smoothly accommodate a charge carrier with relatively large ionic volume in their redox reaction, thereby serving as a suitable electrode active material for Na-ion battery. It is well known that metallic Na reduces ketonic functionality to generate the corresponding ketyl radical, while its great majority are generally transient and simultaneously undergo homo-coupling to give diolate

compounds. One unique exception is fluorenone (**a**) whose ketyl radical (**b**) is stable enough to be isolated, and more significantly, the separately prepared diolate compound (**c**) spontaneously gives rise to the ketyl radical *via* C-C bond fission as shown in Scheme 1^[1].



Therefore, we envisaged that suitably designed organic molecules having multiple fluorenone substructures^[2] undergo multiple redox reaction reversibly to display a high capacity as an electrode active material for Na-ion battery. To verify this hypothesis, we have synthesized the fluorenone derivatives **1–6** (Figure 1) and mixed with acetylene black as a conductive carbon and polytetrafluoroethylene binder in 70:25:5 weight ratios by mortar under air to prepare electrode pellets. Thus fabricated pellets were assembled in 2032 cointype cell with 1 M NaPF₆ in dry EC:DEC = 1:1 as electrolyte, polypropylene as separator (Celgard 3501), and sodium metal as anode under Ar to examine their electrochemical performance. As a result, the compounds **1–6** proved to undergo smooth reversible multiple redox reaction in the solid state but its efficiency may be delicately influenced by the lifetime of their ketyl radicals generated at their discharge termini. For example, truxenone (**6**) showed the initial discharge capacity as high as 190 mAh/g indicative of 2.7 electrons reaction per mole (Figure 2) albeit with a noticeable deterioration upon repeated charge-discharge cycles.



Figure 1. Molecular structure of indenofluorenediones 1–5 (190 mAh/g, 2e/mol) and truxenone 6 (210 mAh/g, 3e/mol).

References:

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