The Critical Role of Fluoroethylene Carbonate (FEC) in the Gassing of Silicon Anodes for Lithium-Ion Batteries

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Silicon (Si) is a promising anode material with high specific capacities (~4000 mA h g^{-1} [$Li_{21}Si_5$], ~3580 mA h g^{-1} [$Li_{15}Si_4$]). However, the pulverization of the Si particles caused by volume changes during (de)lithiation results in poor cycling stability, which has long hindered the implementation of this promising material in next generation lithium-ion batteries. Functionalized electrolytes are effective in mitigating the poor cycling performance, making their investigation essential for the viability of Si.

In this report, we present a comparative study of gaseous byproducts formed by the decomposition of FEC-containing and FEC-free electrolytes using differential electrochemical mass spectrometry and infrared spectroscopy, combined with long-term cycling data of Si half-cells.[1] The evolving gaseous species depend strongly on the electrolyte; the main products for the FEC-based electrolyte are H_2 and CO_2, while the FEC-free electrolyte shows predominantly H_2, C_2H_4, and CO. The evolution characteristics suggest different reactivities of the various Li_xSi alloys. The data acquired from long-term cycling confirm the benefit of using FEC as co-solvent in the electrolyte.

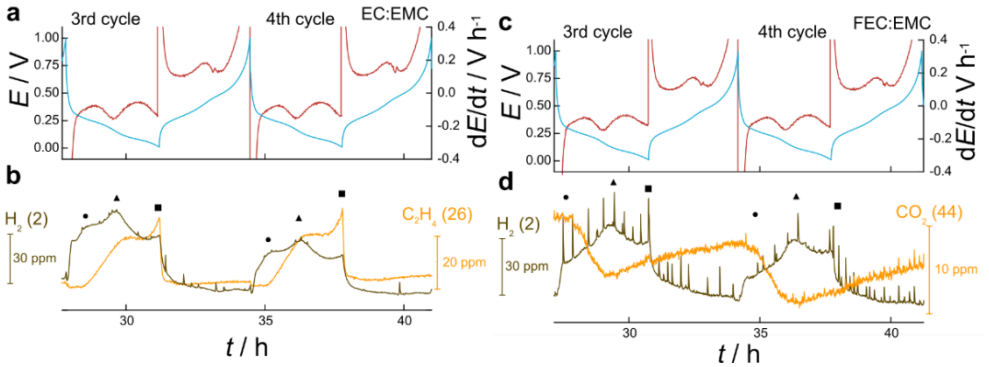

Figure 1. (a, c) Charge/discharge profiles (blue) for the 3rd and 4th cycles and their derivatives (red) of Si half-cells using (a, b) 1 M $LiPF_6$ in EC:EMC and (c, d) FEC:EMC. Characteristic gas evolution pattern of (b) H_2 (brown) and C_2H_4 (orange), and (d) H_2 (brown) and CO_2 (orange).

References:

[1] A. Schiele, B. Breitung, T. Hatsukade, B. B. Berkes, P. Hartmann, J. Janek, T. Brezesinski, ACS Energy Lett. 2 (2017) 2228-2233.