DILITHIUM BENZENEDIPROPIOLATE: A SUPER-LITHIATED ORGANIC ELECTRODE MATERIAL

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Organic electrode materials (OEMs) for lithium-ion batteries (LIBs) constitute a very promising alternative to standard electrodes materials that are prepared from finite and non-renewable minerals resources, but instead being potentially environmental friendly, cheap, and abundant if derived from biomass via ecofriendly processes. However, their commercial use is currently held back due to primarily their poor energy density. High specific capacity OEMs are therefore of high scientific interest. During the last 3 years, OEMs with the ability of an unexpected reversible reduction of carbon-carbon double bonds have sporadically been reported [1]. As a consequence of this redox process – here coined 'superlithiation' – specific energy several times higher than commercial standards (graphite) and Li/C ratios of 1/1 have been reported.

A to-date never reported OEM, dilithium benzenedipropiolate, is here presented [2]. In addition to the expected reduction of its carbonyls, this material can reversibly reduce its unsaturated carbon-carbon bonds leading to a Li/C ratio of 1/1 and specific capacity as high as 1363 mAh g^{-1}: the highest ever reported for a lithium carboxylate. Density functional theory calculations suggest that the lithiation is preferential on the propiolate carbons. Due to that the sp hybridized carbons in this material are reacting according to the 'super-lithiation' mechanism, a path for design of OEMs able of Li/C ratios as high as 2/1 has been opened up.

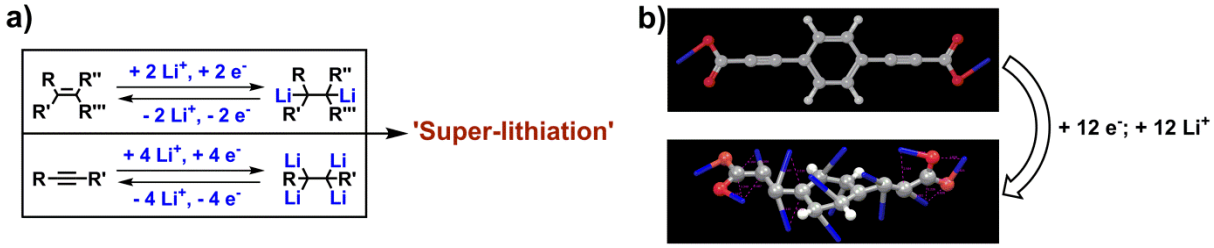

Fig. 1 a) 'Superlithiation' mechanism. b) Proposed lithium insertion mechanism in dilithium benzenedipropiolate.

[1] a) X. Han, G. Qing, J. Sun, T. Sun, Angew. Chem. Int. Ed., 51 (2012), 5147. b) W. Luo, M. Allen, V. Raju, X. Ji, Adv. Energy Mater., 4 (2014), 1400554. c) J. Wu, X. Rui, C. Wang, W.-B. Pei, R. Lau, Q. Yan, Q. Zhang, Adv. Enegy Mater., 5 (2015), 1402189. d) J. Wu, X. Rui, G. Long, W. Chen, Q. Yan, Q. Zhang, Angew. Chem. Int. Ed., 54 (2015), 7354.

[2] S. Renault, V.A. Oltean, C.M. Araujo, A. Grigoriev, K. Edström, D. Brandell, submitted.