Graphene doping as a way to improve electrochemical properties of Li-S batteries

Saioa Zorita
Francisco Fernández-Carretero
Inés Rincón
Yolanda Belaustegi
Alberto García

Materials for Energy and Environment Area, TECNALIA, Parque Científico y Tecnológico de Gipuzkoa, E-20009 San Sebastian-Donostia, Spain

Saioa.zorita@tecnalia.com; francisco.fernandez@tecnalia.com

Abstract

Nowadays there is an increasing demand for high energy storage systems and Li-S batteries are considered one of the most promising technologies with a high theoretical specific capacity of 1675 mAh/g and high theoretical specific energy of 2600 Wh/kg.

In order to reach the theoretical specific capacity, there are issues that must be overcome. The principal challenges regarding the Li-S cathode are the poor conductivity of sulphur, the dimensional change during cycling and the polysulphides shuttle.

Reduced graphene oxide (rGO) has a strong effect on the suppression of the polysulfide shuttle increasing the cycling stability. Asymmetric charge distribution, created by e.g. doping of graphene oxide (GO) with heteroatoms (N, B, S etc.), affects the polarity and thus creates sites for binding polysulphides.

It is possible to self-assemble the 2D-GO on a 3D-rGO structure. This 3D-rGO enables a stable pathway for electron percolation while the polysulphides can be retained by the polar groups present on the surface of the rGO. Moreover, 3D-rGO can be filled up with high contents of sulphur, leading to the manufacture of more “realistic” electrodes with higher energy densities.

In this work various simple routes of N, B and S rGO-doping, were investigated to improve the electrochemical performance (electrical conductivity and cycling performance). These materials were characterized by FT-IR and Raman spectroscopy indicating the functionalization of the GO with N, B and S.

These doped 3D-rGO (Fig. 1) materials were loaded with up to 99.5% elemental sulphur to be used as cathodes for Lithium-sulphur batteries, resulting on sulphur content on the cathode of 80% (w).

The first results suggested that N and S doping offered the best electrochemical characteristics. Highest electrical conductivity was obtained when doping with thiourea (up to 19 S/cm). Furthermore the sulphur/N-S doped 3D-rGO composite showed an enhanced cycling performance as seen in Fig 2. (650 mAh/g after 50 cycles at 0.1C rate).

Figures

Figure 1: 3D-r GO

Figure 2: Discharge capacity of N, S doped rGO and B doped rGO at C/10