Selenium-doped graphene nanoplatelets for energy storage

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In this study, we investigated the effects of selenium doping in reduced graphene oxide (rGO) and energy storage performances of the selenium-doped rGO (Se-rGO). Numerous selenium atoms were homogeneously doped on the top surface of rGOs; it caused little structural change, indicative of surface transfer doping. High-resolution TEM images showed no aggregates or nanoparticles on the surface of rGOs, indicating that selenium atoms were introduced in an atomic level. Based on first principles calculations, we found the selenium atoms to be mainly bonded to the surface edge defect sites of highly amorphorized rGO, leading to the enhancement of electrical conductivity due to n-type doping. In contrast, the overall intrinsic topological defects of the graphene basal plane showed an unfavorable selenium atom binding energy. The doped selenium atoms changed the electrical transport properties of rGO. The properties were well fitted by the fluctuation-induced tunneling mechanism, and the results indicated the presence of a large metallic region separated by a relatively small insulating gap. The σ value of Se-rGO reached 210 S cm^{-1} at 300 K, while the $\sigma/\sigma_{20\ K}$ parameter was almost constant (1.3-fold increase from 20 to 300 K), this indicated that the carrier mobility of Se-rGO was similar to that of graphene. In addition, Se-rGO showed a superior electrochemical performance as an anode for Li-ion batteries, exhibiting ~570 mAh g^{-1} at a current density of 1 C (372 mA g^{-1}). In a low-temperature cell test, the reversible capacity of Se-rGO is ~360 mAh g^{-1}, corresponding to ~ 63% of the capacity at 25 °C. In contrast, rGO shows a reversible capacity of ~140 mAh g^{-1}, corresponding to ~ 45% of that at 25 °C. These results suggest that the enhanced electrical properties of Se-rGO affect its electrochemical performance at low temperature to a great extent. Moreover, highly stable capacities of 165 mAh g^{-1} could be obtained at a large current rate of 50 C, which is approximately seven times higher than the value of rGO anode materials.