

Lithium storage mechanisms of CdSe nanoparticles with carbon modification for advanced lithium ion batteries

Experimental

Synthesis

Graphene oxide (GO) was prepared using the modified hummer's method [39]. The carbon nanotube (CNT) was functionalized with concentrated HNO₃ before synthesis. 40 mg GO or CNT was dispersed in 60 ml deionized water under ultrasonication for 0.5 h to form carbon suspension. 2 mmol Cd(NO₃)₂·4H₂O and 4 mmol SeO₂ were added into this dispersion with constant stirring for 0.5 h. Then, 10 ml hydrazine hydrate (N₂H₄·H₂O, 50 %) was added into this dispersion with constant stirring for another 0.5 h. The mixture was pulled in a 100 ml Teflon-lined stainless steel autoclave and heated at 180 °C for 24 h. After reaction, CdSe/reduced Graphene oxide and CdSe/Carbon nanotube composites were finally obtained after repeated washing with deionized water and drying at 60 °C overnight in a vacuum oven, which were named as CdSe@rGO and CdSe@CNT, respectively. CdSe nanoparticles were prepared under the same procedure without adding GO and CNT.

Characterization

The phase of samples were characterized by powder X-ray diffraction (XRD) on a Rigaku X-ray diffractometer (Dmax-2200) with a scan rate of 4°/min. Raman spectra were recorded on Raman spectrometer (Thermo Fischer DXR). The carbon content in the CdSe@rGO and CdSe@CNT composites were determined using thermogravimetric analysis (TGA, STA449F3C) at a heating rate of 10 °C min⁻¹ under O₂ gas atmosphere. The morphologies and microstructure of samples were observed using field emission scanning electron microscopy (FESEM, SIGMA), transmission electron microscopy (TEM, JEOL-2000CX) and high-resolution TEM (HRTEM, JEOL-2010F). The chemical valences of atoms for samples were collected by X-ray photoelectron spectrometer (XPS, Thermo ESCALAB 250Xi).

Electrochemical measurement

The working electrodes on copper foil consisted of 80 wt% active materials, 10 wt%

acetylene black and 10 wt% polyvinylidene. The typical loading mass of active material is $\sim 2.1 \text{ mg cm}^{-2}$ and the thickness of electrode is $\sim 150 \text{ }\mu\text{m}$. The coin cells were assembled using lithium foil as the counter electrode and Celgard 2500 membrane as the separator. The electrolyte is 1 M LiPF_6 solution in ethylene carbonate, dimethyl carbonate and ethyl-methyl carbonate with a volume ratio of 1:1:1. Galvanostatic charge and discharge tests were performed on a LAND CT2001A. Cycle voltammetry (CV) at various scan rates and electrochemical impedance spectroscopy (EIS) between 10 mHz and 100 kHz were carried out using the VSP electrochemical workstation (Biologic, FRA).

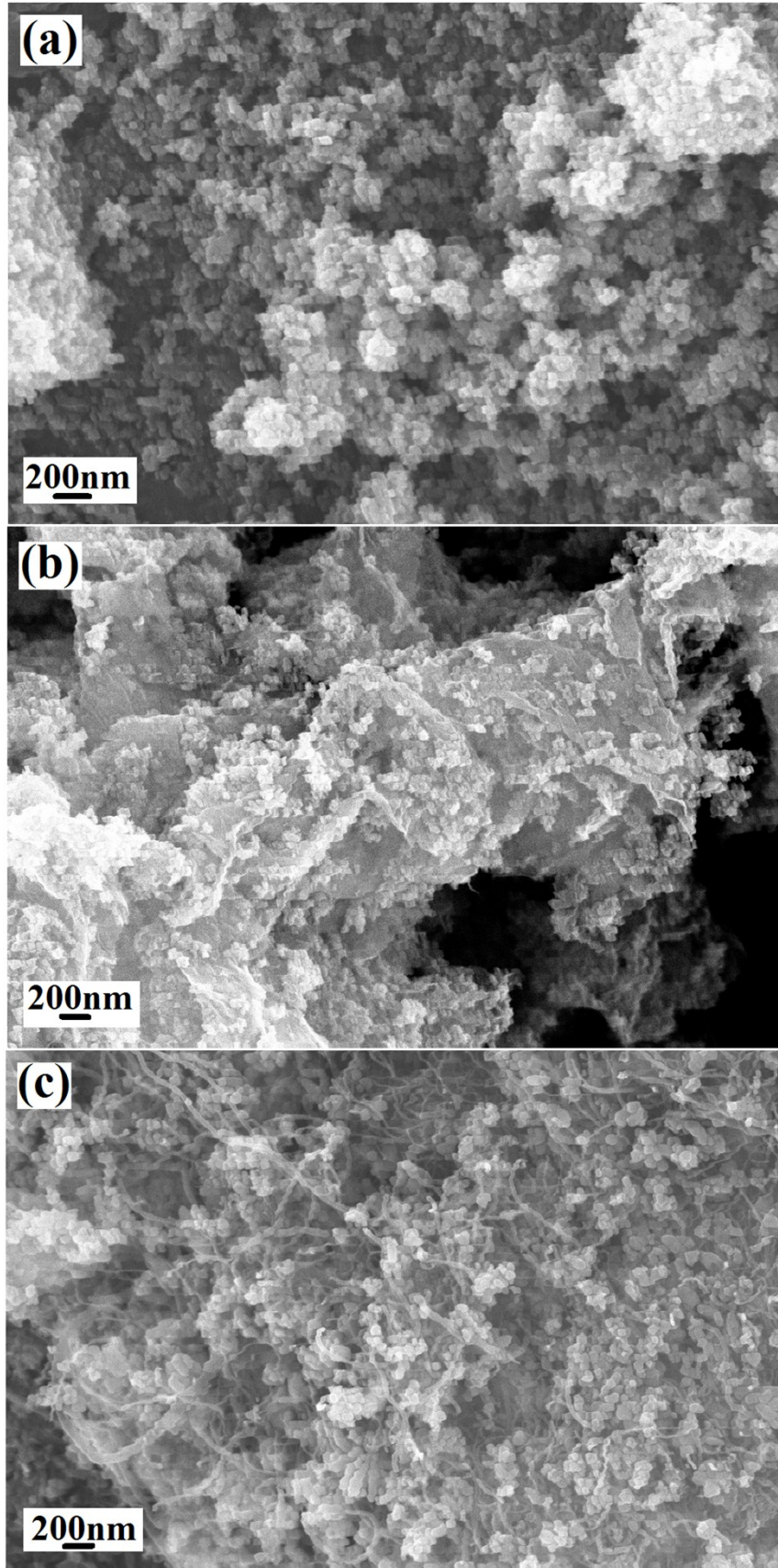


Fig. S1. High magnification SEM images of (a) CdSe, (b) CdSe@rGO and (c) CdSe@CNT.

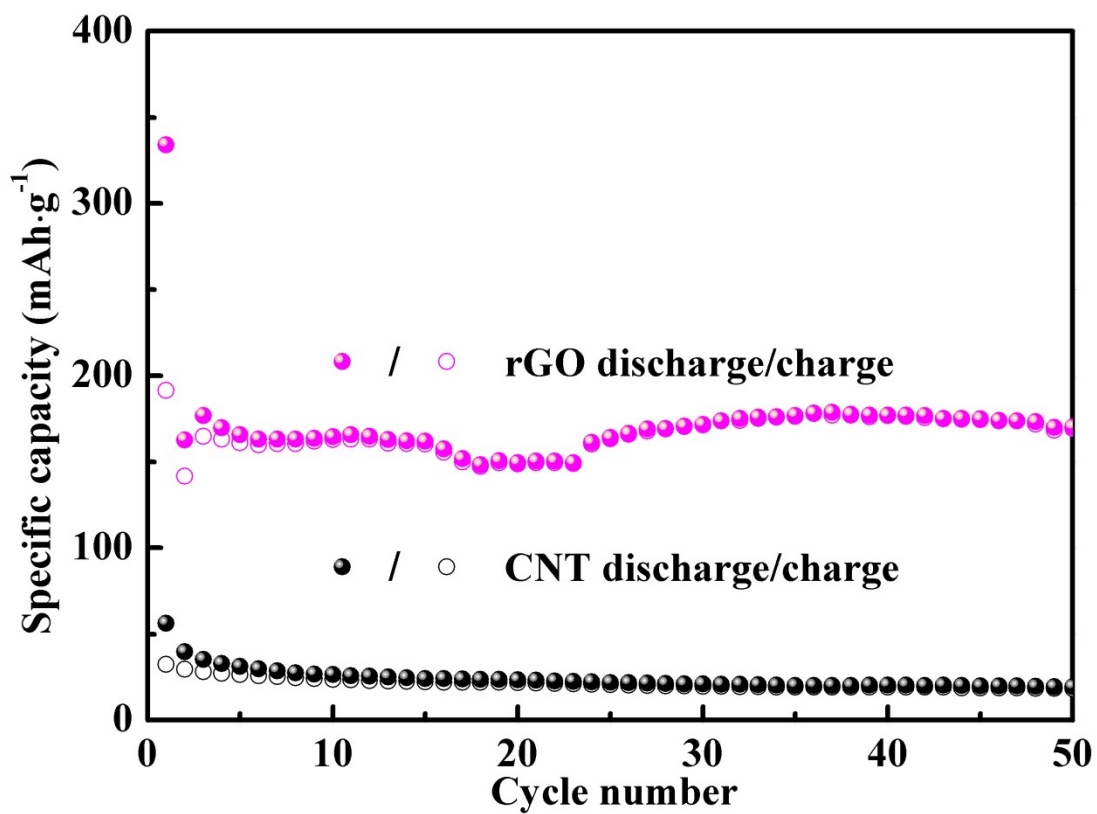


Fig. S2. Cycling performance of rGO and CNT at 100 mA g^{-1} .

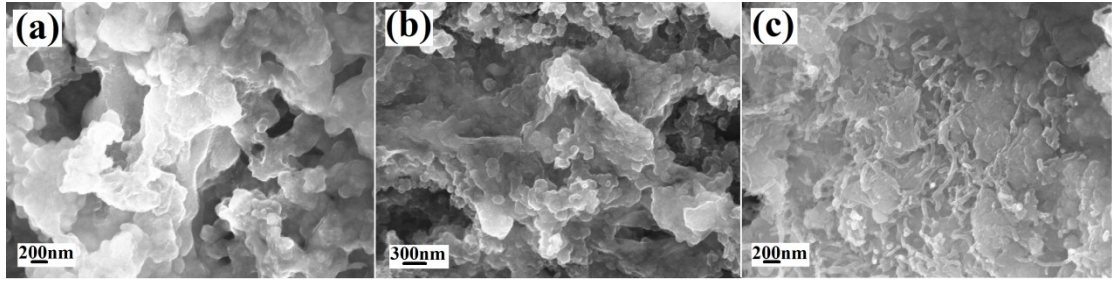


Fig. S3. High magnification SEM images of (a) CdSe, (b) CdSe@rGO and (c) CdSe@CNT after 10 cycles.

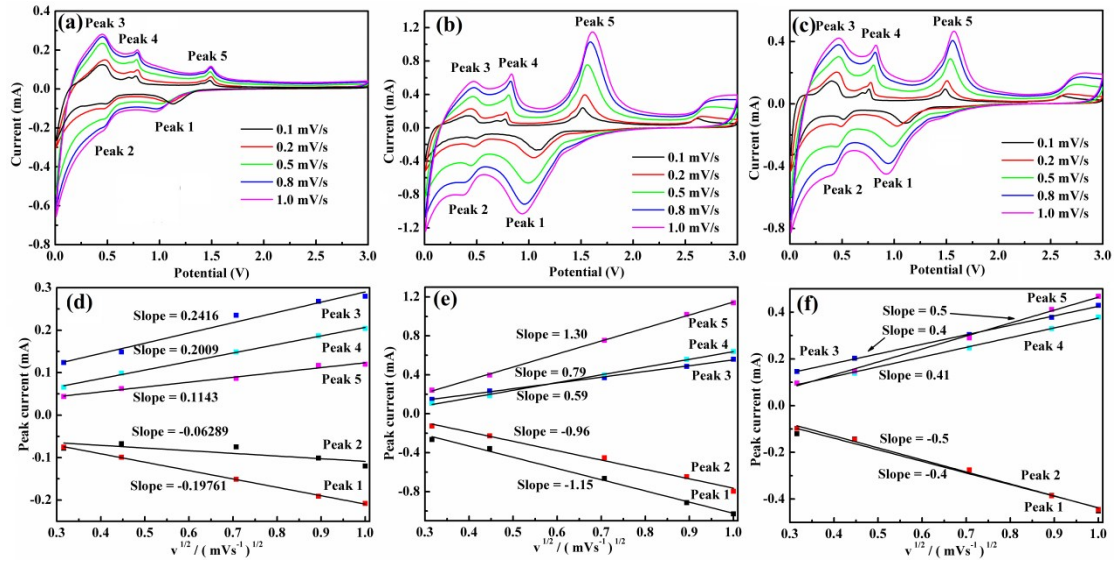


Fig. S4. CVs of CdSe (a), CdSe@rGO (b) and CdSe@CNT (c) electrodes at different scan rates; The peak current against the square root of scan rates for the CdSe (d), CdSe@rGO (e) and CdSe@CNT (f) electrodes.

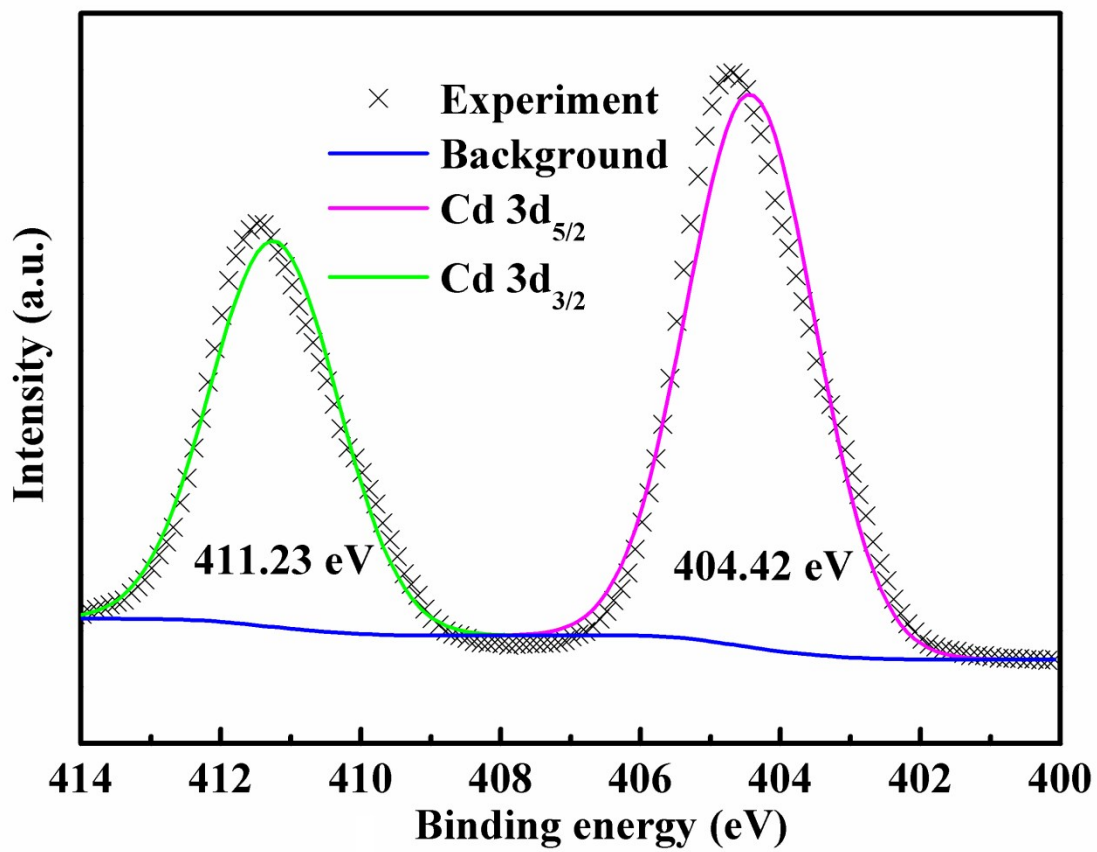


Fig. S5. XPS spectrum of Cd powder.

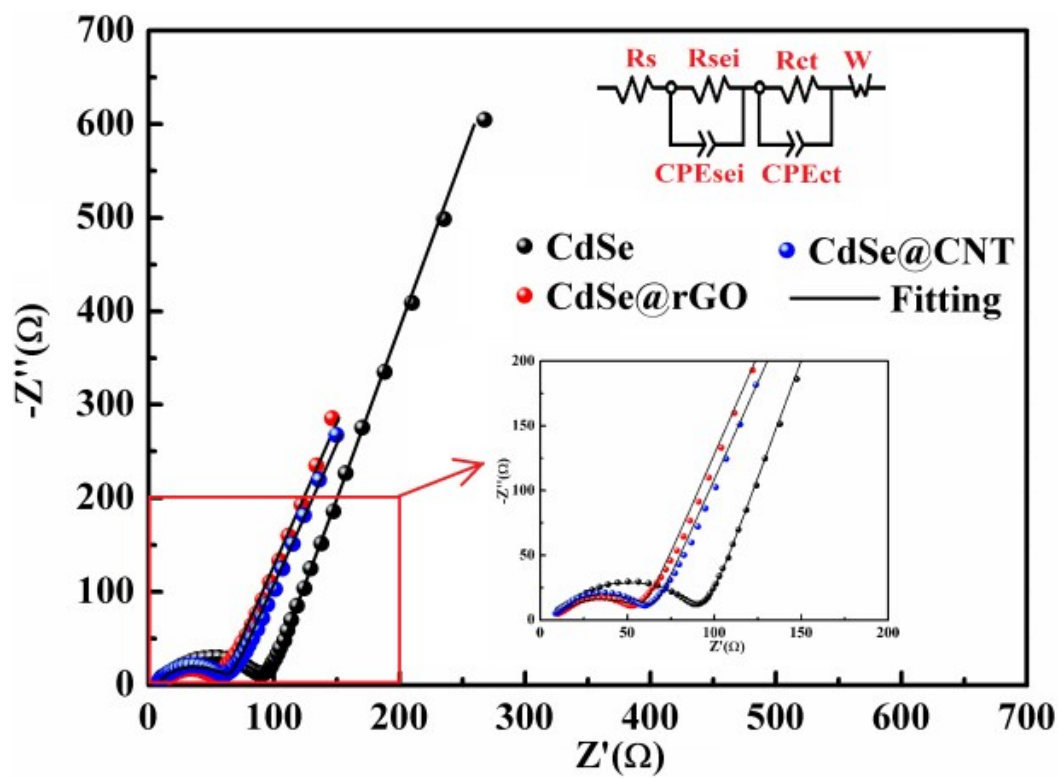


Fig. S6. Nyquist plots of the cells of the CdSe, CdSe@rGO and CdSe@CNT electrodes after 10 cycles.