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Effect of the redox reactivity of vanadium ions enhanced by phosphorylethanolamine based catalyst on the performance of vanadium redox flow battery



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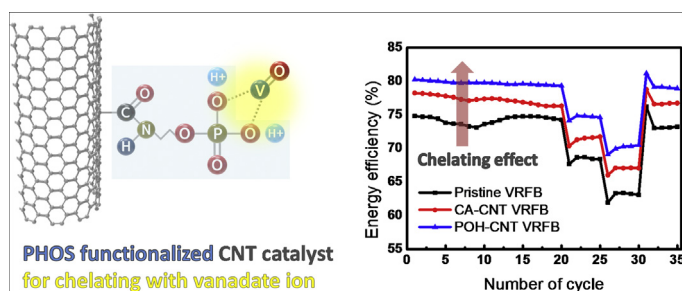
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HIGHLIGHTS

- Phosphorylethanolamine doped carbon nanotube (POH-CNT) is suggested as catalyst.
- POH-CNT exhibits superior catalytic activity for $\text{VO}^{2+}/\text{VO}_2^+$ redox reaction.
- Chelation ability of phosphate group promotes $\text{VO}^{2+}/\text{VO}_2^+$ redox reaction rate.
- Electron delocalization capability and acid dissociation constant are key factors.
- Performance of VRFB single cell using POH-CNT catalyst is improved.

GRAPHICAL ABSTRACT



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ABSTRACT

Phosphorylethanolamine (PHOS) doped carbon nanotube (CNT) is newly suggested as a catalyst for enhancing the redox reactions of vanadium ions and vanadium redox flow battery (VRFB) performance. For synthesizing the catalyst, CNT is linked to the phosphate group of the PHOS, forming phosphate functionalized carbon nanotube (POH-CNT). Its catalytic activity is then compared with those of pure CNT and carboxylic acid functionalized CNT (CA-CNT) catalysts. Regarding the redox reactivity of vanadium ions, POH-CNT exhibits superior catalytic activity and reaction reversibility for $\text{VO}^{2+}/\text{VO}_2^+$ reaction to CNT and CA-CNT because of (i) the chelation ability of phosphate group, (ii) its low electron delocalization capability and (iii) its high acid dissociation constant. By the role as chelating agent of phosphate group, the density of active sites for reaction of VO^{2+} and VO_2^+ ions in POH-CNT increase. Also, the low electron delocalization and high acid dissociation constant induce effective adsorption and desorption of VO^{2+} and VO_2^+ ions. Such effects facilitate the $\text{VO}^{2+}/\text{VO}_2^+$ reaction. In contrast, regarding $\text{V}^{2+}/\text{V}^{3+}$ reaction, POH-CNT shows equivalent reactivity to CA-CNT because phosphate and carboxyl groups form similar active sites for the $\text{V}^{2+}/\text{V}^{3+}$ reaction. The above results are supported by calculating kinetic parameters, such as charge transfer resistance and diffusion coefficient, while chemical bonding of the catalysts is examined by XPS. Finally, as the POH-CNT is used as catalyst for positive electrode prompting the $\text{VO}^{2+}/\text{VO}_2^+$ reaction, performance of VRFB single cell is improved.

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