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### Multifunctional Conformal Polymer Coating By Oxidative Chemical Vapor Deposition for High Specific Energy Ni-Rich Cathode

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#### Abstract Text:

The successful commercialization of lithium-ion batteries (LIBs) leads to wide utilization in portable electronic devices such as cellphones and laptops because of their excellent cycle performance and moderate rate capability [1]. Technical challenges still remain to enhance specific energy of LIBs to be implemented in large-scale devices including hybrid electric vehicles (HEVs) and electric vehicles (EVs) [2]. Adopting high specific capacity electrode materials and decreasing the weight ratio of non-capacity materials in batteries are considered as two main methods for improving the overall specific energy for LIBs.

Ni-rich layer oxides as one of the mainstream cathode materials have drawn much attention due to their high theoretical specific capacity. However, the surface and bulk degradation of Ni-rich materials during circulation may trigger capacity loss and generate serious safety issues, which limits its application in LIBs [3]. Coating inert inorganic compounds has been suggested to enhance the stability of Ni-rich materials. However, it is also reported that the coating layer was delaminated from the cathode bulk particles due to the anisotropic volume change during lithiation and delithiation as well as the stiff nature of inorganic coating materials [4].

On the other hand, reducing non-capacity materials such as conductive carbon led to the lower electronic conductivity, which may cause polarization and increase the resistance of the battery. Meanwhile, a traditional binder is electronically insulating, limiting electron transportation. In addition, less binder in electrodes could result in separation of the active materials from the electrode, causing battery capacity loss [5].

In order to accommodate the volume variation during circulation, polymers with resilience possibly protect the Ni-rich particles during cycle life. Further, binders and conductive carbonaceous are preferred to construct conductive networks for electrodes for enhancing the overall conductivity of the battery. As thus the polymer with electronic conductivity is supposed to be uniformly coated on Ni-rich particles and sufficiently distributed in the electrode.

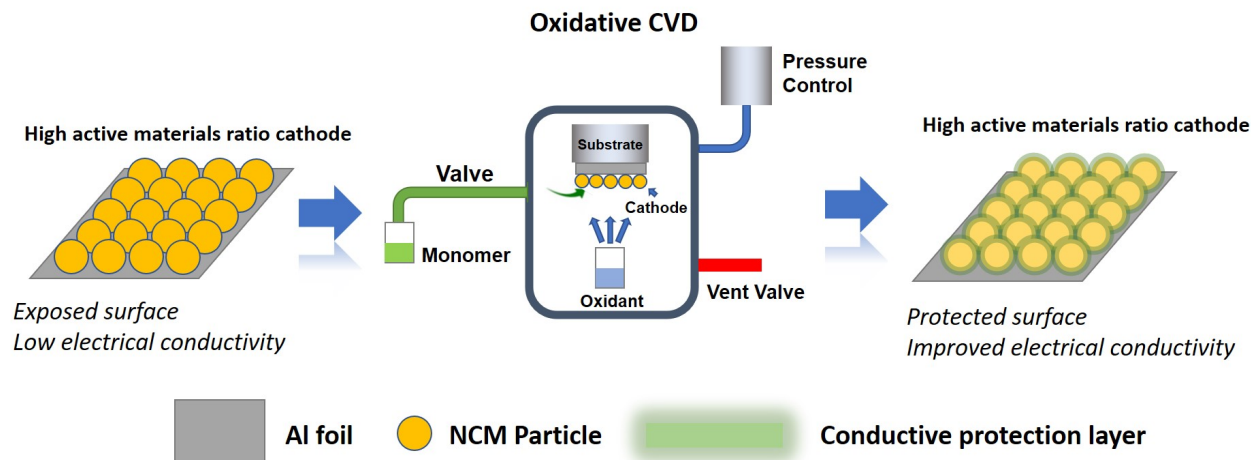
Poly(3,4-ethylenedioxythiophene) (PEDOT) is a promising polymer due to its high electrical conductivity and the demonstrated protection ability for Ni-rich materials in LIBs [6]. Meanwhile, as an emerging technique, oxidative chemical vapor deposition (oCVD) is a deposition process that generates uniform and conformal polymers via gas phase reaction with a vaporized source monomer (in this case EDOT) and an oxidizer (in this case  $\text{FeCl}_3$ ). PEDOT deposited on the electrode through the oCVD method is homogeneous on the surface of Ni-rich particles. And the high electronic conductivity of the polymer would enhance the battery performance as well as the adhesive ability of the polymer own.

In this study, Ni-rich cathode with 99% active materials weight ratio was prepared from as-synthesized  $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$  (NCM811) particles and oxidative chemical vapor deposition method was employed to generate a controllable PEDOT layer with 55 nm thickness. Moreover, the PEDOT layer was found between the secondary particles, indicating excellent conformal coating capability of the oCVD technique. Further characterization X-ray photoelectron spectroscopy (XPS) and Density functional theory calculation (DFT) revealed that sulfide in PEDOT is preferentially bonded with transition metal (Ni, Co and Mn) in NCM811, which prolonged the service life of the PEDOT layer. Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) and XPS was employed which unveiled the formed PEDOT layer restricted the parasite reaction during the charge/discharge process and diminished the transition metal dissolving, and endowed the battery with improved stability (81.6% after 300 cycles under 1C,  $1\text{C} = 200\text{ mA g}^{-1}$ ) Cyclic voltammetry (CV) showed less difference value for modification sample ( $\Delta E = 0.14\text{ V}$ ) compared with pristine sample ( $\Delta E = 0.25\text{ V}$ ).

Furthermore, the battery even showed  $171.5\text{ mAh g}^{-1}$  under 7C and high reversibility after a high rate, which provides a potential for the fast-charge. The trifunctional PEDOT layer is verified to serve as the protection layer, binder and electronic conductivity network for the cathode materials. The results of this study demonstrate significant promises of employing the high active material weight ratio with high cycle life and a pathway for various kinds of cathode materials for reaching higher specific energy as well.

## Reference:

- [1]. Goodenough, J. B.; Park, K. S., J Am Chem Soc 2013, 135 (4), 1167-76.
- [2]. Lee, W.; Yoon, W.-S., Advanced Energy Materials 2018, 8 (4), 1701788.
- [3]. Sun, Y. K.; Myung, S. T.; Park, B. C.; Prakash, J.; Belharouak, I.; Amine, K., Nat Mater 2009, 8 (4), 320-4.
- [4]. Liu, J.; Manthiram, A., Journal of The Electrochemical Society 2009, 156 (1).
- [5]. Jeong S.S., Journal of Power Source 2012, 199 (1).
- [6]. Xu G.-L.; Chen G., Nature Energy 2019, 4.

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