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# Designing Nanostructure Material to Achieve High Energy Density Li-metal Battery

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**Abstract:** Lithium-sulfur (Li-S) battery with high theoretical energy density of 2600 Wh/kg, expected to be next generation battery technology. In reality polysulfide formation, shuttling effect, low conductivity of Sulfur and low active material loading become major challenges to develop Li-S battery technology. Here, we design a bilayer separator, consists of molybdenum oxide nanobelts (MoO<sub>3</sub> NB) prepared by facile physical grinding process, coated onto Celgard separator to mitigate shuttling effect. Li-S battery using modified separator exhibit initial capacity of 679 mAh/g with degradation rate of 0.014% per cycle and capacity retained 29.4% after 5000 cycles at 5C rate. Easy fabrication approach, good mechanical strength and extraordinary cycle performance using modified separator can offer scalable solution for future commercial Li-S battery application.

# Scheme Polysulfide Repulsion $2Li + S_8 \leftrightarrow Li_2S_8$

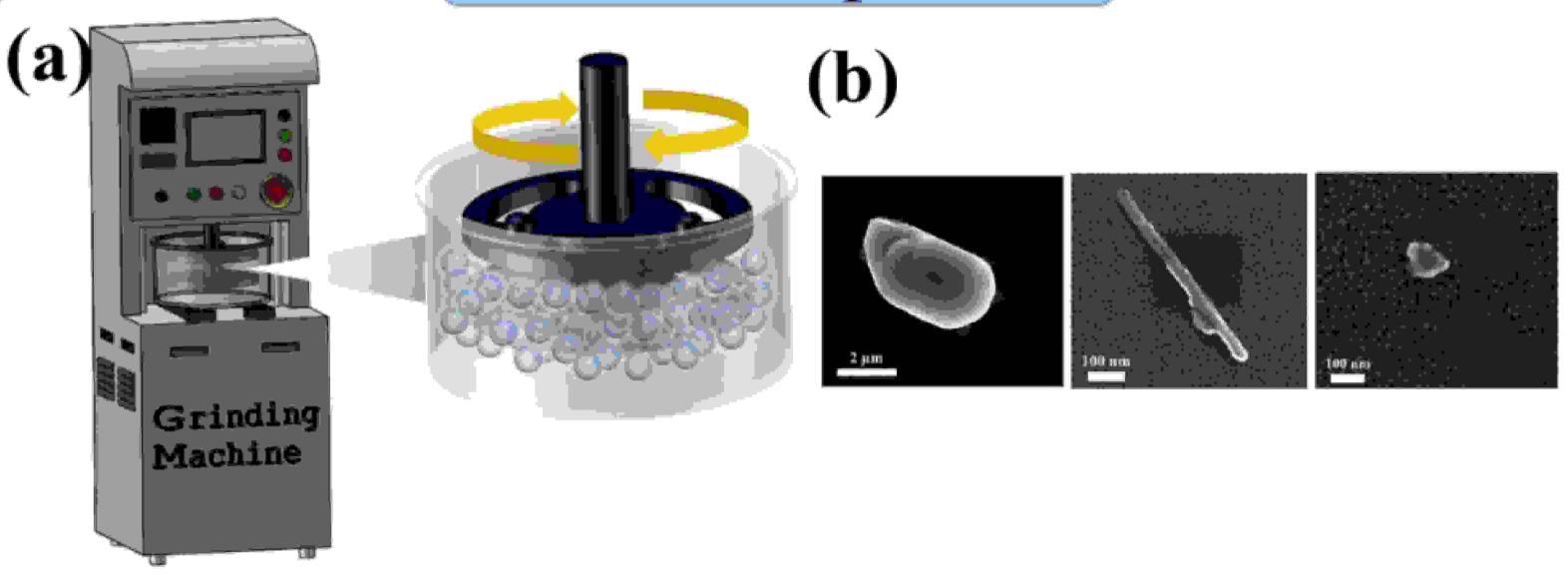
**Scheme 1.** Schematic representation of Li-S battery using MoO<sub>3</sub> NB coated separator and trapping of polysulfides

# Fig 3. Polysulfide diffusion test using (a) pristine separator and (b) MoO<sub>3</sub> NB

Polysulfide diffusion test

coated Separator

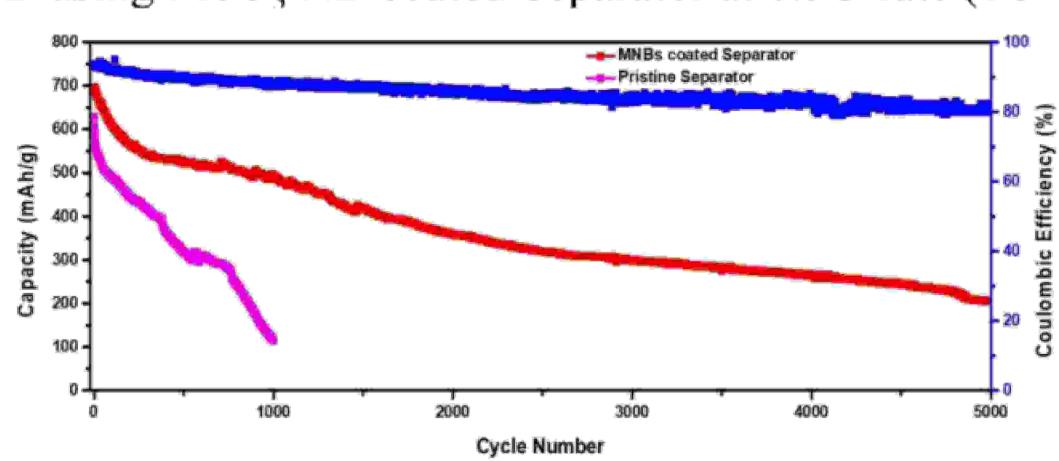
### Material Preparation



**Fig 1.** (a) Schematic diagram of homemade grinding machine (b) FESEM image of bulk, Nanobelt and nanoparticle MoO<sub>3</sub> prepared by grinding method.

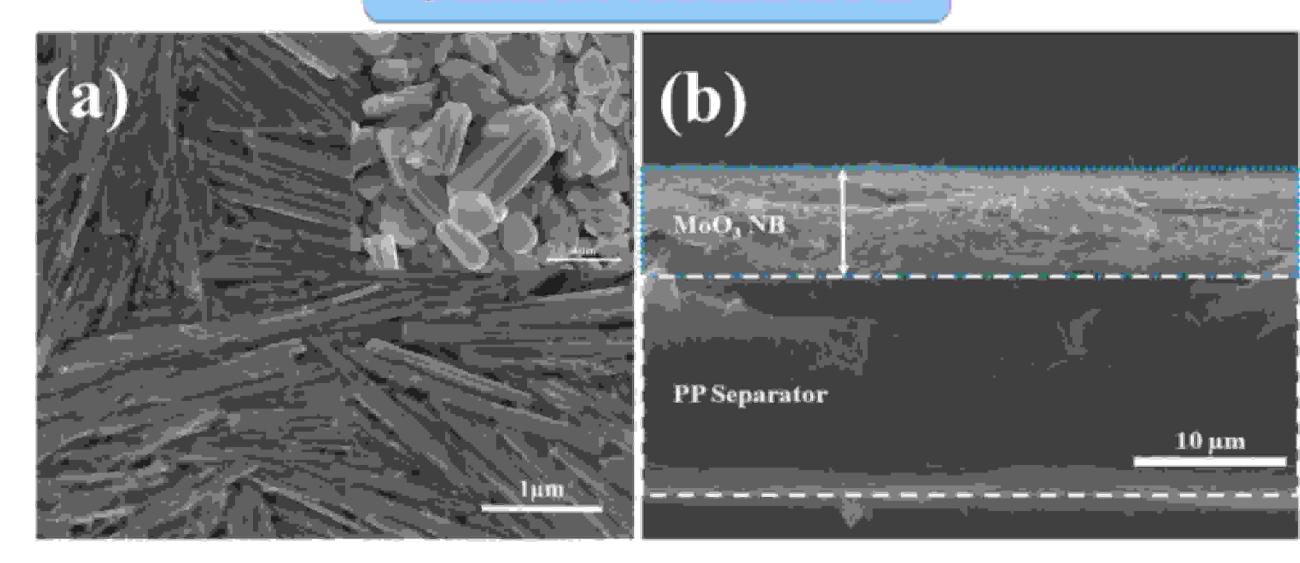
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**Fig 4.** (a) Cyclic voltammetry curve and (b) galvanostatic charge-discharge profile of LSB using MoO<sub>3</sub> NB coated Separator at 0.5C-rate (1C=1675 mAh/g).



**Fig 5**. Long-term Cycling performance of LSB using MoO<sub>3</sub> NB coated Separator at 5C-rate.

#### Characterization



**Fig 2.** (a) FESEM images of MoO<sub>3</sub> NB prepared by grinding (inset: commercial MoO<sub>3</sub> bulk) and (b) cross-sectional SEM image of MoO<sub>3</sub> NB coated PP separator

Published in *Nanoscale*, 2019 11(6), 2892-2900.

### Conclusion

We develop a bilayer separator by coating MoO<sub>3</sub> NB onto commercial Celgard separator, which provides physical and chemical interaction with polysulfides to mitigate the shuttle phenomenon to a greater. Finding of this facile design has potential for commercialization of functional separator for Li-S battery to mass production at low cost.

Patent: Taiwan, US (Pending)

