

# Molecular Design Strategies to Achieve High Voltage and Energy Organic Electrode Materials for Secondary Batteries

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## Abstract

With emerging demand for sustainable and green energy storages, organic electrode materials have attracted much attention as promising alternatives to the conventional metal-oxide ones due to their potential advantages in low-cost, natural abundance, environmental friendliness, and easy chemical tunability. A lot of organic redox-active molecules have been reported as electrode materials for metal-ion secondary batteries so far. Although they have demonstrated promising performance particularly in terms of high specific capacity and cyclability, their redox potentials lie mostly between 3.0 and 1.0 V vs. Li/Li<sup>+</sup>, which are still inferior to the inorganic electrode materials. In this talk, we present novel molecular design strategies to tune the redox potentials of organic redox-active molecules for achieving high energy electrode materials in Li- and Na-ion batteries.

First, we will demonstrate a simple molecular design strategy to raise the redox potential of quinone derivatives which is one of the most promising ones among the reported organic electrode materials. By substituting electron-withdrawing halogen atoms into p-benzoquinone (BQ), we could lower its lowest unoccupied molecular orbital (LUMO) energy where the electrons are inserted during the reduction process, which led to redox potential increase (~2.9 V vs. Na/Na<sup>+</sup> and ~3.1 V vs. Li/Li<sup>+</sup>).[1]

Next, to achieve both large specific capacity and high energy, we developed a new molecular design strategy using a triptycene scaffold as a minimal linker.[2] The triptycene molecule bearing three BQs in a rigid tripod structure delivered a specific capacity of 387 mAh/g and a specific energy of 1032 Wh/kg in Li-ion cells. Its large capacity and high energy were attributed to the 3-D arrangements of BQ units in the triptycene structure, which not only facilitated multi-electron redox reaction but also raised its redox potential.

Finally, we will discuss the effect of substituting functional groups on the redox potential of disodium terephthalate (Na<sub>2</sub>TP) derivatives.[3] It is shown that the strong binding interaction between the charge carrying ions (Li<sup>+</sup>) and methoxy substituents significantly lowers the free energy of the discharged products and thus resulting in redox potential increase, which is contrary to the prior knowledge that electron donating groups generally lowers redox potential of organic electrode materials.

We believe that these findings can provide important guidelines to finely tune the charge/discharge voltage of new organic electrode materials.

**Keywords:** Redox-active Molecules, Organic Electrode, Organic Battery, Secondary Battery

## References

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## Biography

Ji Eon Kwon received his BS and Ph. D degree in Materials Science and Engineering (MSE) from Seoul National University (SNU) in 2006 and 2014, respectively. He was appointed Korea Presidential Post-doc. Fellow in 2016. He is currently a Research Assistant Professor at the Research Institute of Advanced Materials (RIAM), SNU since 2016. His current research topics are mainly focused on the development of organic materials for various types of secondary batteries.