Abstract Submitted
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**Structural Stability and Electronic Properties of $Na_2C_6O_6$ for a Rechargeable Sodium-ion Battery**[1] TOMOKI YAMASHITA, Kyoto University, AKIHIRO FUJII, HIROYOSHI MOMIDA, TAMIO OGUCHI, Osaka University — Sodium-ion batteries have been explored as a promising alternative to lithium-ion batteries owing to a significant advantage of a natural abundance of sodium. Recently, it has been reported that disodium rhodizonate, $Na_2C_6O_6$, exhibit good electrochemical properties and cycle performance as a minor-metal free organic cathode for sodium-ion batteries. However, its crystal structures during discharge/charge cycle still remain unclear. In this work, we theoretically propose feasible crystal structures of $Na_{2+x}C_6O_6$ using first principles calculations. A structural phase transition has been found: $Na_4C_6O_6$ has a different $C_6O_6$ packing arrangement from $Na_2C_6O_6$. Electronic structures of $Na_{2+x}C_6O_6$ during discharge/charge cycle are also discussed. Our predictions could be the key to understanding the discharge/charge process of $Na_2C_6O_6$.

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