MERIT Internship Report

Department of chemical system engineering, School of engineering

MERIT 8th

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1. Period

From November 1st, 2021 to November 30th, 2021

2. Hosting company

Murata Manufacturing Co., Ltd. Minato MIRAI Innovation Center

Battery development department, Device center, Corporate Technology & Business Development Unit

3. Theme

The effect of elements doping in $LiCoO_2$

4. Contents of research

Background

The upper voltage cutoff of $LiCoO_2$, the most important cathode material for lithium-ion batteries, has increased to 4.45 V from 4.2 V in recent 30 years, which resulted in the growth of its energy density. Further charging to above 4.5 V leads to significant capacity fade in cycling, although the higher cutoff is necessary to achieve more increased energy density. This is mainly caused by the phase transition, where Co layers glide on each other.

In this research, the effect of elements doping on the phase transition in $LiCoO_2$ is studied by theoretical calculations.

Methods

PBE-D3 function was used for first-principal calculation of materials. Cluster expansion was used for delithiated structures and large supercells including more than 100 atoms. Monte Carlo simulation was used for finding optimal arrangement of atoms.

Results

The phase transitions in pure $LiCoO_2$ and $LiCoO_2$ with the substitution of Co for a certain transition-metal element (*M*-doped $LiCoO_2$) were compared in theoretical calculations. Although *M* doping seemed to suppress the phase transition in previous reports, the structure after the phase transition was more stable in *M*-doped $LiCoO_2$ in the calculation using small supercells including about 50 atoms. Then, the theoretical model where the local arrangements of atoms suppress the phase transition was suggested because these factors were not considered in the previous calculation with small supercells. This theory was verified in the calculation with large supercells with about 2000 atoms using Monte Carlo simulation and cluster expansion method.

5. Acknowledgements

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