COMPUTATIONAL MODELLING OF LI-ION CARBOXYPHENOLATE-BASED ELECTRODE MATERIALS

AUTHORS

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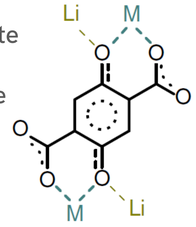
INTRODUCTION

- Green and environment-friendly storage devices are needed. Lithium-ion batteries are well established but are harmful to the environment due to the metals present in the electrodes.
- The molecule (2,3-dilithium-oxy)-terephthalate is a good alternative to the current materials. It also showed a high potential as an electrode material, even more when combined with "spectator cations" - here denoted as M.

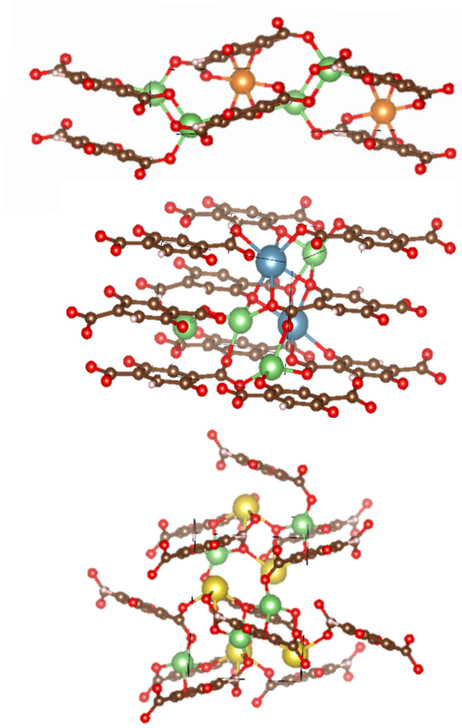


OBJECTIVE

- Predict crystal structures for the electrode materials: composed by the ligand DHT (oxy-terephthalate), Lithium ions and the spectator ions: Mg+2, Na+, Ca+2.
- Study voltage profile of each material.
- Understand the voltage difference by studying and simulating the electronic structure.
- Understand the charge profile by Bader analysis.

RESULTS/FINDINGS

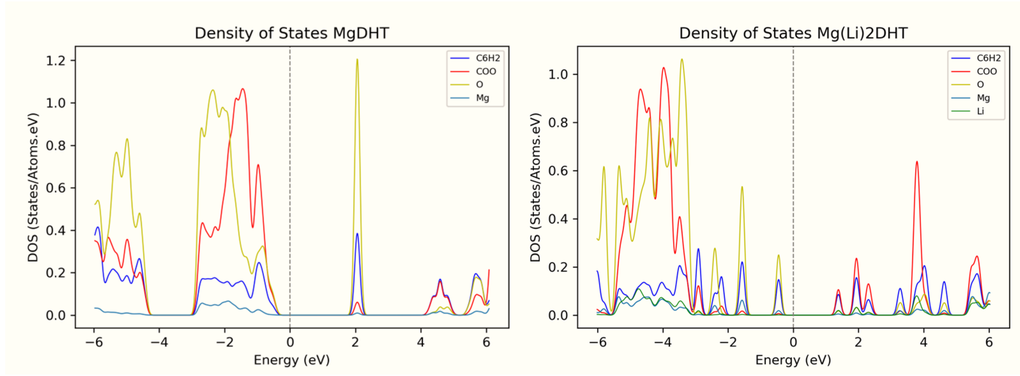
STRUCTURE AND VOLTAGE PREDICTIONS



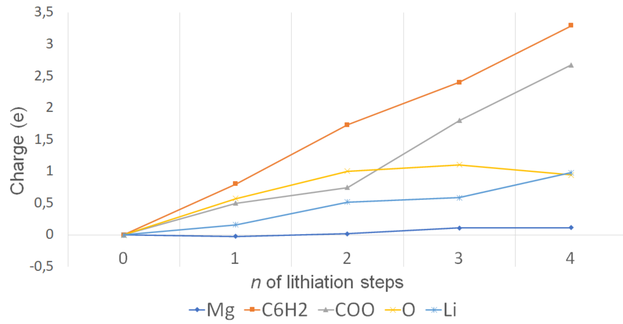
MgLi2DHT
~3.59V

Na2Li2DHT
~2.96V

CaLi2DHT
~2.98V



BADER ANALISYS



METHODOLOGY

Molecular modelling:
(Magnesium, sodium, calcium)
(2,5-dilithium-oxy)-terephthalate.

Crystal Structure predictions:
USPEX software
(Evolutionary algorithm).

Electronic structure calculations with VASP :
•DFT-based code
•GGA/PBE xc functional
•HS06: Hybrid functional

CONCLUSION

- Without no experimental input, voltage predictions agree to experimental results.
- We successfully predicted the materials structures.
- By changing the spectator cation, we were able to analyze the electronic structure and understand the tendencies of the material.
- The charge profile showed how different cations affect how charge is distributed during the lithiation process.

REFERENCES

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