PAUL SCHERRER INSTITUT

ELECTROCHEMISTRY LABORATORY

BATTERIES

Lithium iron methylene diphosphonate, a new organic-inorganic hybrid positive electrode material for Li-ion batteries

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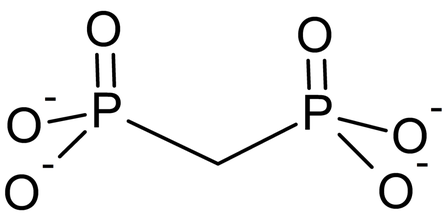
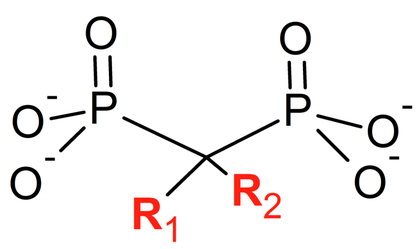
Methylene diphosphonate

- Ligand for organic-inorganic hybrid materials
- Alternative to carboxylic acid groups as ligands as used in other hybrid battery materials
- Varying substituents (R_1, R_2) → quasi-infinite possibilities to design new materials

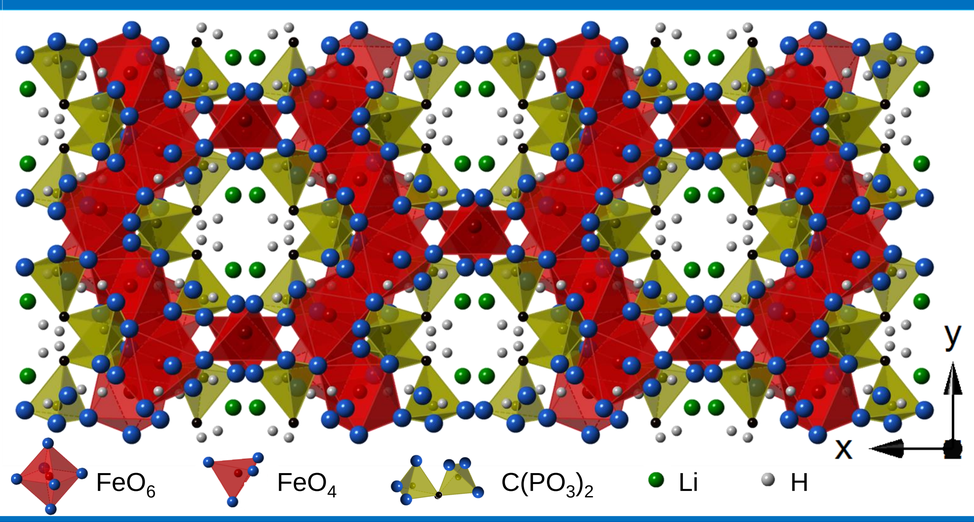
Methylene diphosphonate:

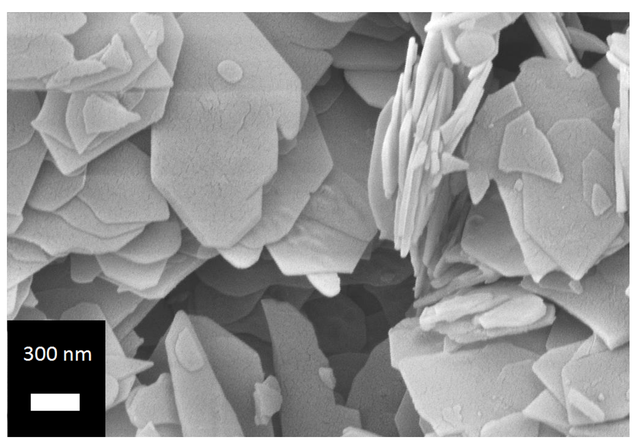


Perspective:



Structure & morphology





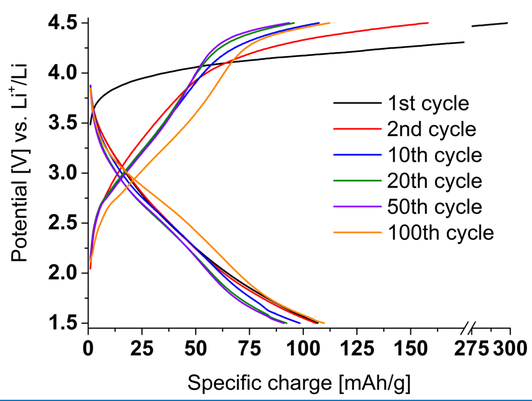
Refined structure:

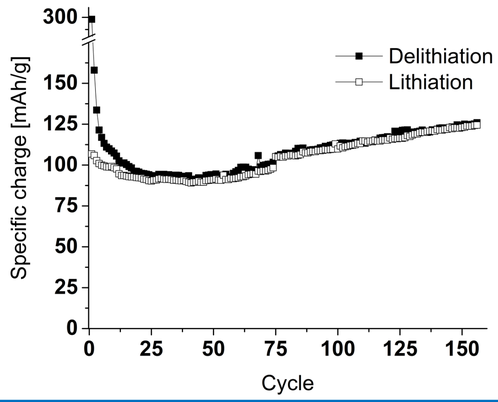
- Monoclinic space group
- Octahedrally and tetrahedrally coordinated Fe sites
- Li sites located in channels

SEM:

- Sub-micrometric platelets, 40 – 50 nm thickness

Electrochemical properties

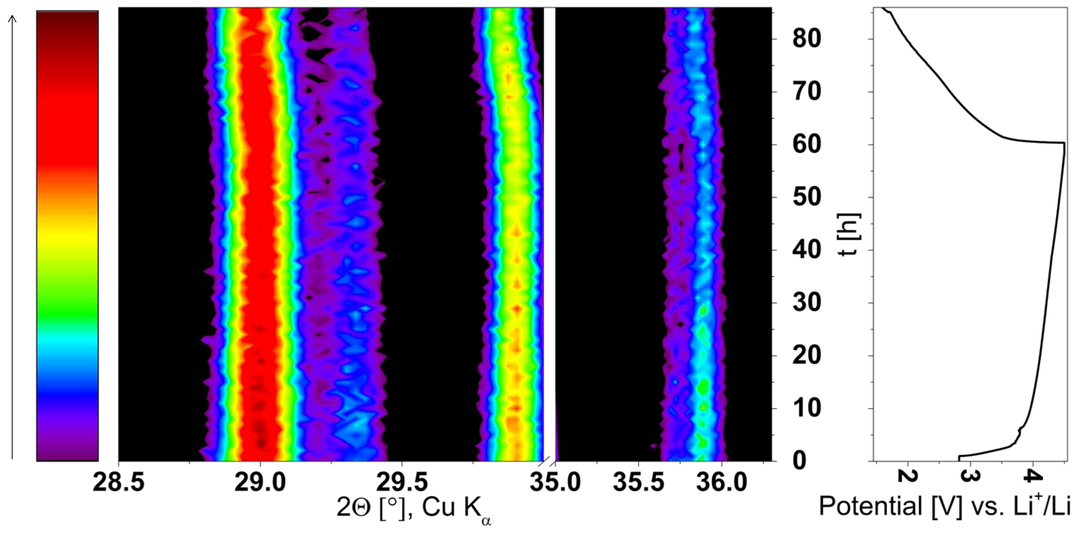




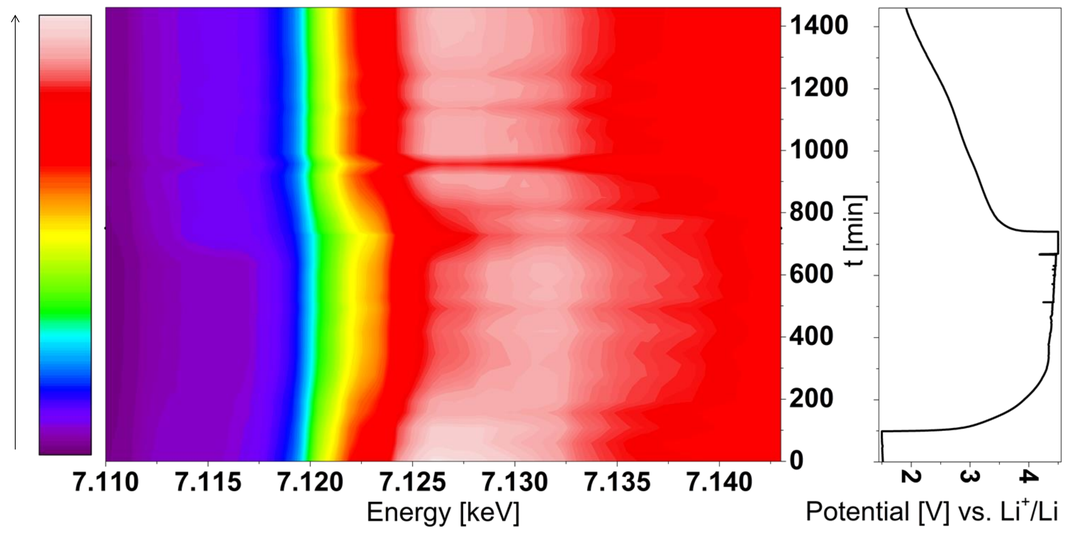
- Increase in specific charge after 60 cycles, slight change in galvanostatic profile → suspected change in morphology [1].
- Ex situ IR (not shown) → diphosphonate still present after 40 cycles.

[1] Wang et al., *Advanced Energy Materials*, **2013**, *3*, 606 – 614.

In situ XRD / in situ XANES



XRD: Only small change in the unit cell parameters



XANES: Fe(II) ↔ Fe(III) reversible cycling

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Conclusions

- Lithium iron methylene diphosphonate can be cycled in half-cells
- Channels allow Li insertion/extrusion without strong disturbance of the unit cell parameters
- Results submitted for publication