PAUL SCHERRER INSTITUT

ELECTROCHEMISTRY LABORATORY

BATTERIES

Lithium Iron Diphosphonates, Organic-Inorganic Hybrid Materials as New Positive Electrode Materials for Li-Ion Batteries

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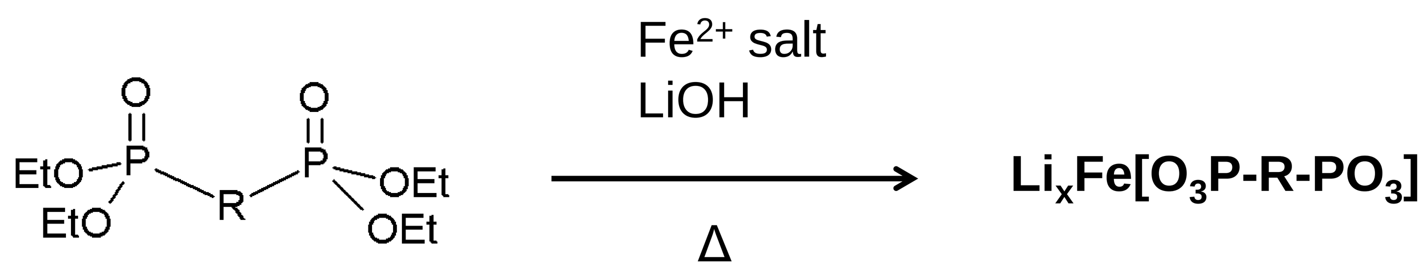
Why organic-inorganic hybrids?

To combine:

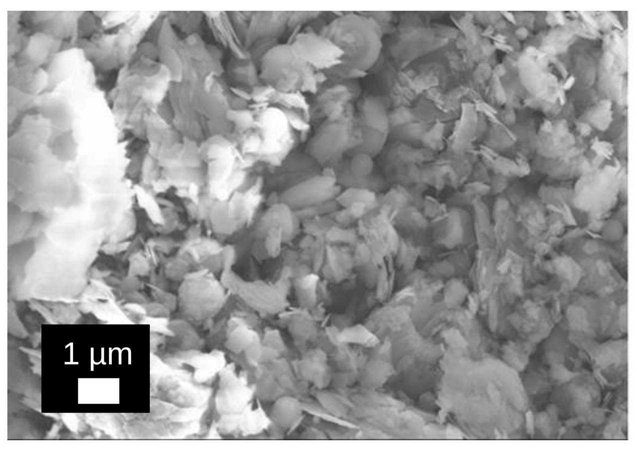
- Cycling stability similar to inorganic materials
- Easy and fast synthesis
- Varying organic part **R** → quasi-infinite number of materials accessible
- → Proof of concept: Lithium metal diphosphonates **$Li_xM[O_3P\text{-}R\text{-}PO_3]$**
- → targeted model material **$Li_xFe[CH_2(PO_3)_2]$**

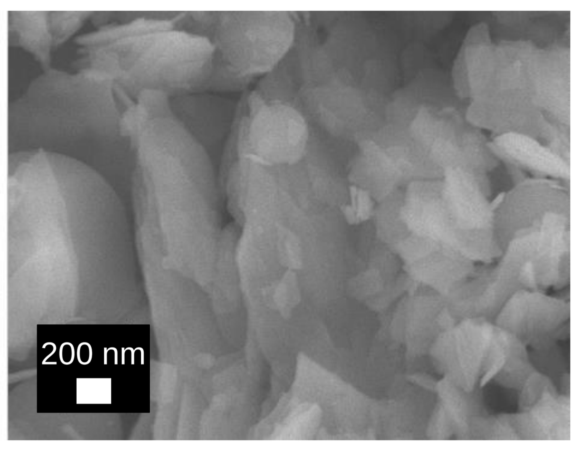
Synthesis



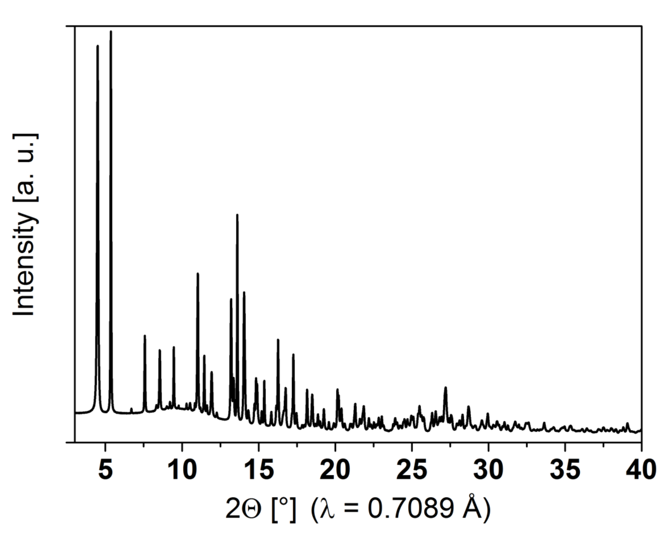
R = CH_2, C_2H_4, $CH(NMe_2)$

Characterization (R = CH_2)

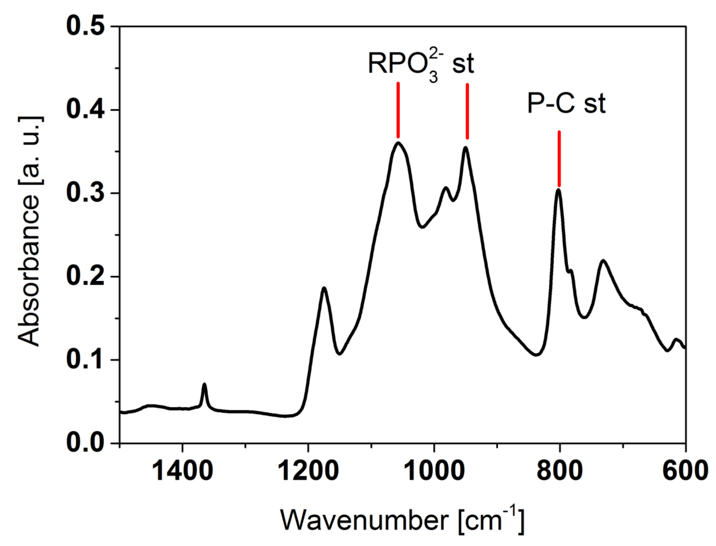




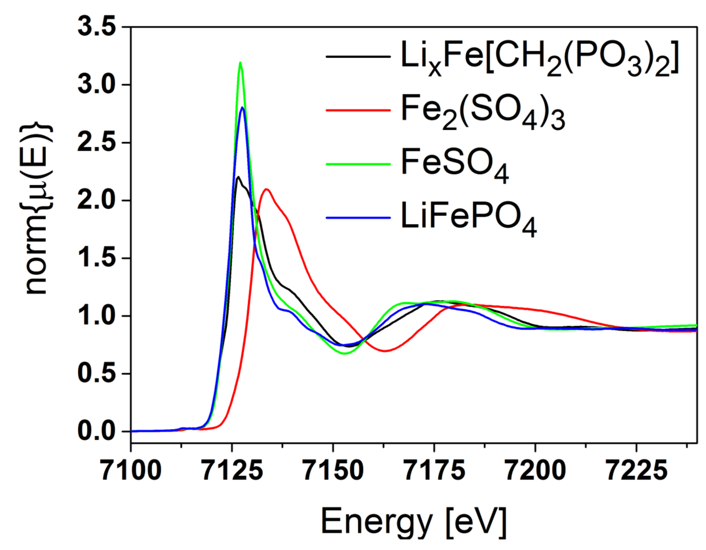
SEM → thin platelet-shaped particles with a dimension of roughly 0.5 µm



X-ray diffraction → crystalline product, probably monoclinic

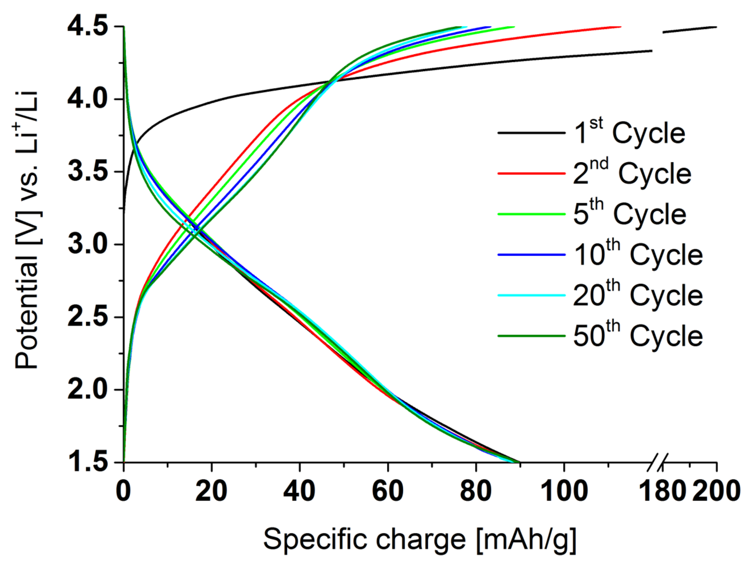


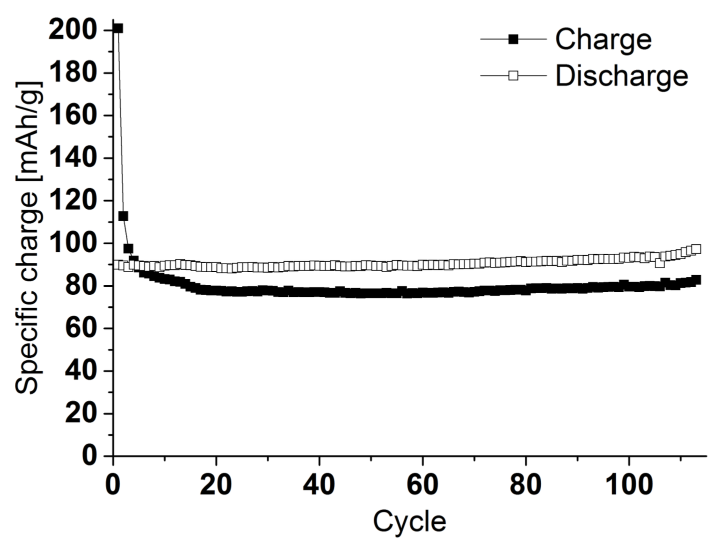
FT-IR → diphosphonate



XANES → mainly Fe^{2+}

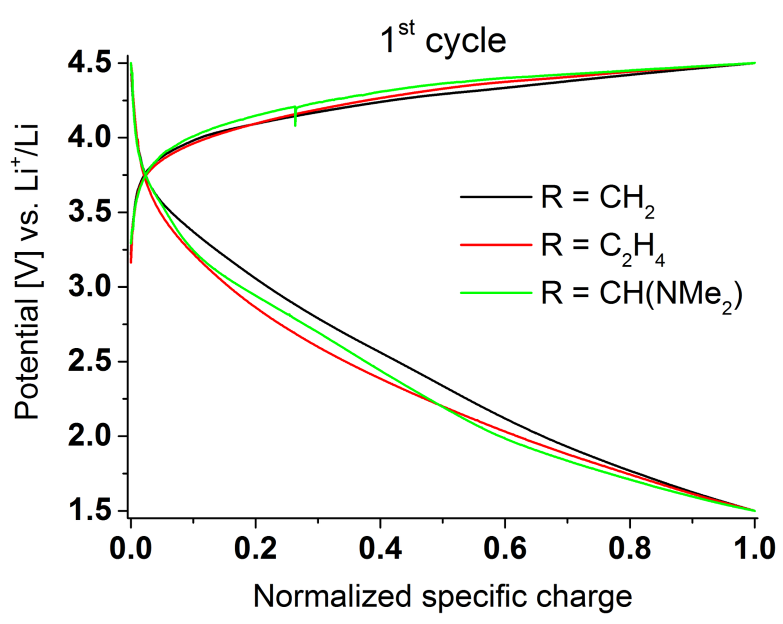
Electrochemistry (R = CH_2)



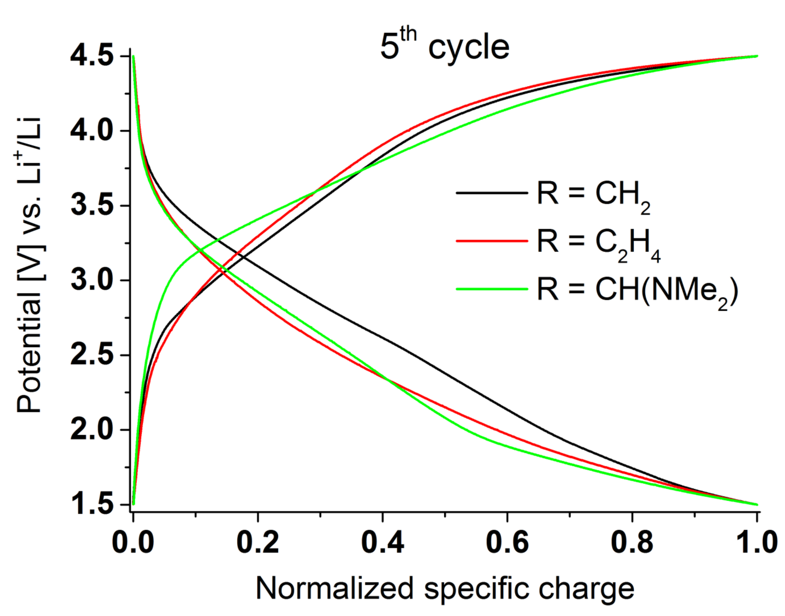


- Stable specific charge for more than 100 cycles
  - $C_{discharge, stable}$ ≈ 90 mAh/g
  - $C_{theoretical}$ ≈ 110 mAh/g
- Stabilization of profile after 20 cycles
- Large irreversibility during first charge → SPI? Activation of electrode material?
- Ex situ IR (not shown) → diphosphonate still present after 40 cycles

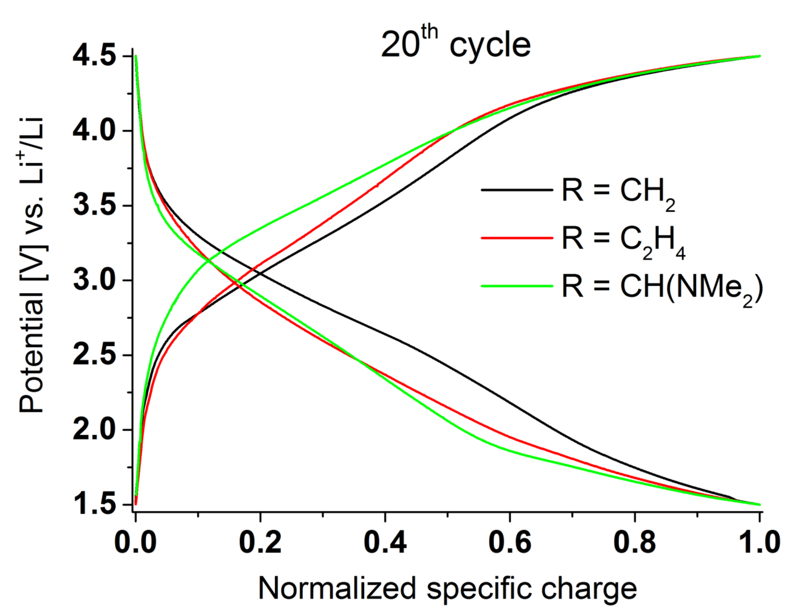
Influence of the organic component R



1st cycle:
Similar potential profile for all R-groups



5th cycle:
Different electrochemical properties are observable for the different R-groups



20th cycle:
Strongest change of potential profile for R = Me, smallest for R = $CH(NMe_2)$

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Conclusions

- Metal diphosphonates can be synthesized and used as positive electrode materials in Li-ion batteries
- Diphosphonates seems to be stable under cycling conditions
- Varying R can change the electrochemistry