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Nanomaterials of Lithium Iron Alkoxides for Use in Lithium Ion Batteries

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1815 – Inorganic Chemistry and Nanomaterials

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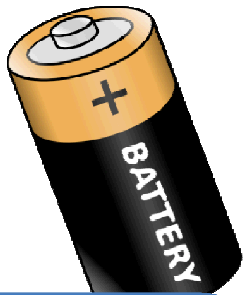
Li-Ion Batteries (LIB)differ from classical batteries by transporting a Li ion reversibly



Battery definition: cells (independent or connected) that produce a current by converting chemical energy to electrical energy

Parts of a Battery

a. Cathode

b. Separator (Electrolyte)

a. Anode

LIB have widespread use but many improvements are still necessary

- Used Everywhere
  - i.e. phones, laptops, cars, etc.

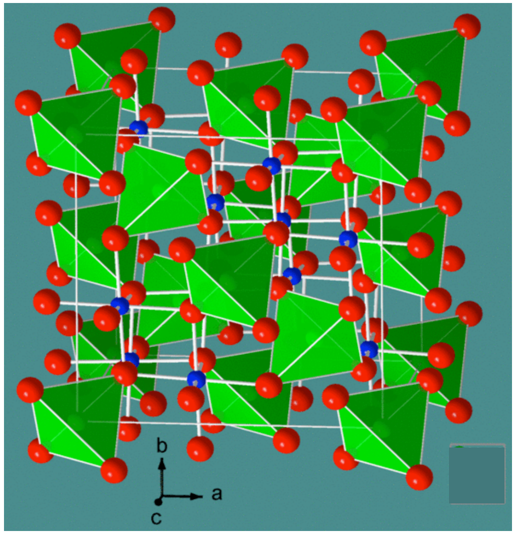
- Issues
  - Mechanical Degradation
  - Short life span





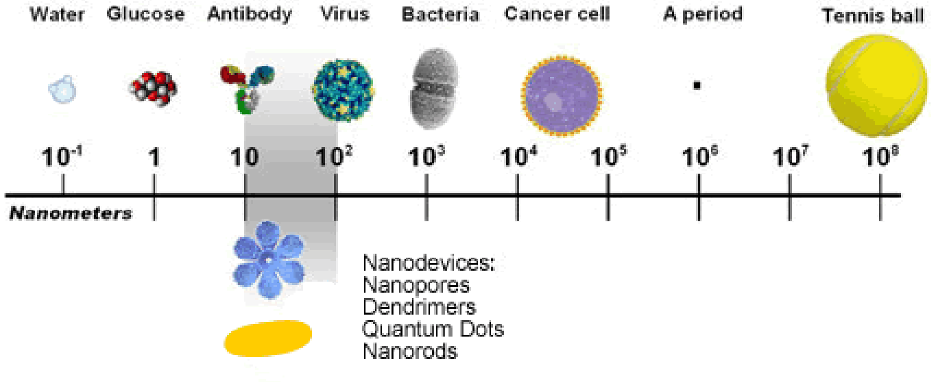
Determine Performance of nanomaterials of the $LiFeO_x$ spinel phase as Lithium Ion cathode materials.

- Develop novel precursors using iron lithium alkoxides
- Develop routes to nanomaterials using iron lithium alkoxides
- Test nanomaterials for use in Li-Ion Battery batteries



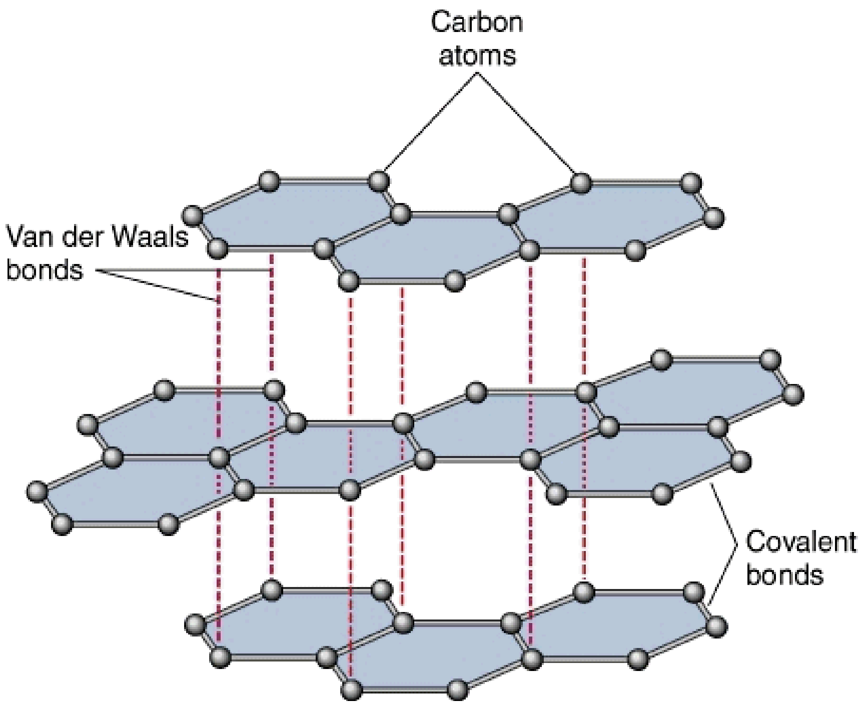
Metal alkoxide: proton on an alcohol replaced by a metal.

Nanomaterials: Materials with morphological details on the nanoscale.

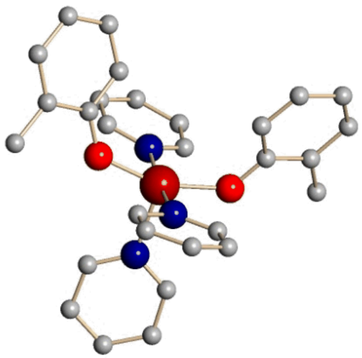


Moving to the nanoregime promised to overcome some of the bulk material limitations

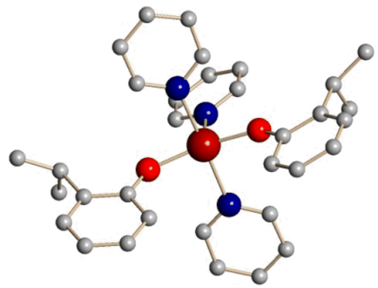
- New properties encountered at this scale
- More surface area = more room for reactions
- High surface area = more stability during charge/discharge



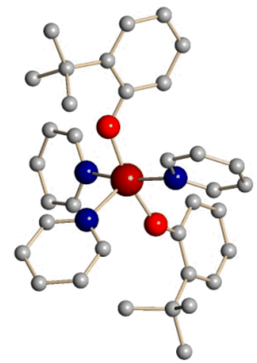
Novel iron alkoxides were investigated for nanomaterial production



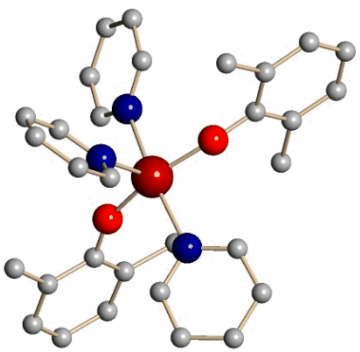
9fb253: $Fe(omP)_2(py)_3$



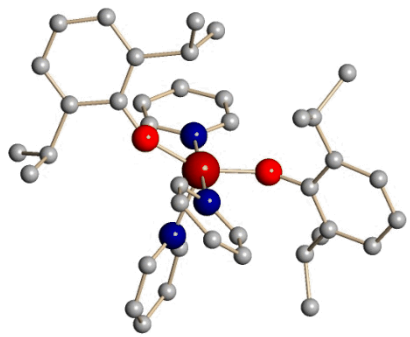
9jy172: $Fe(oPP)_2(py)_3$



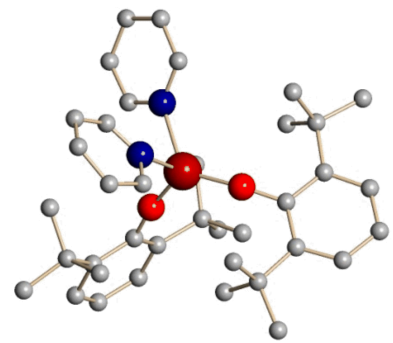
9jn042: $Fe(oBP)_2(py)_3$



9nv241: $Fe(DMP)_2(py)_3$



9nv251: $Fe(DIP)_2(py)_3$

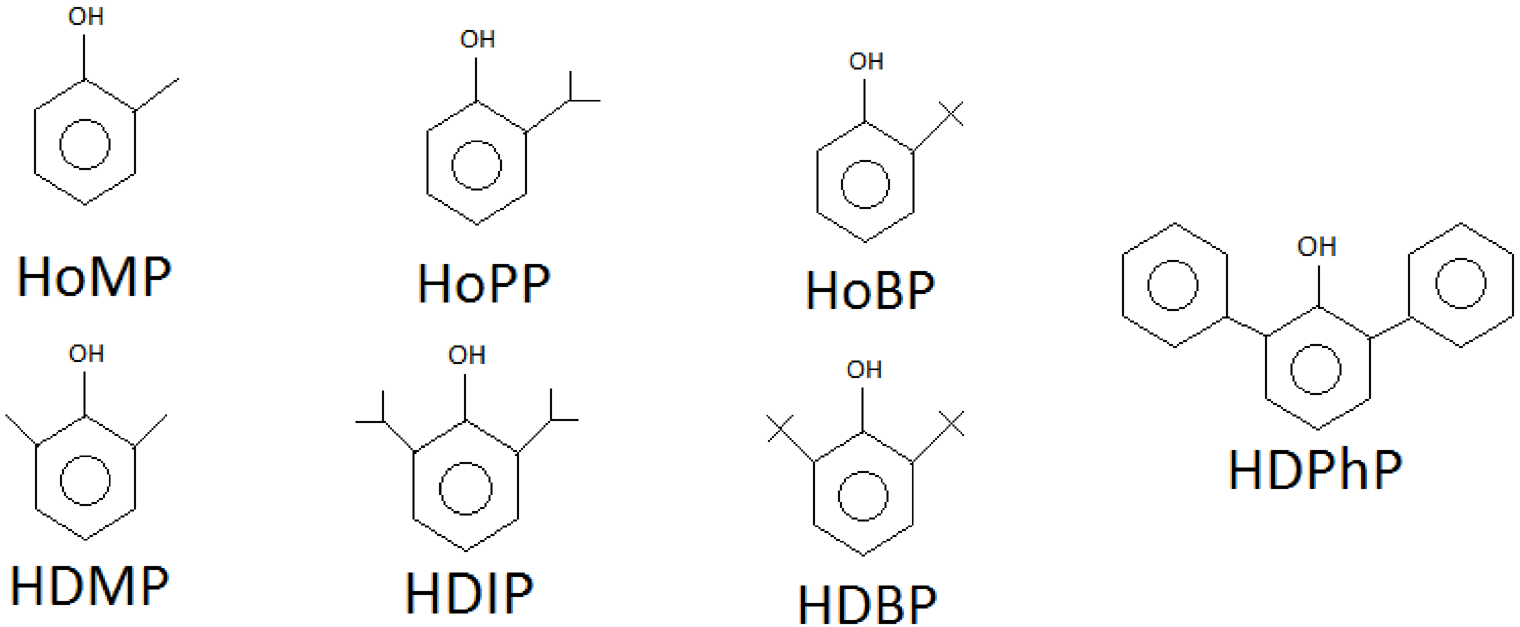


9jn081: $Fe(DBP)_2(py)_2$

Timothy J. Boyle, et al. Inorganic Chem. 2011.

Will single-source precursors to $LiFeO_x$ be more useful than the FeOx nanomaterials

$$\mathbf{Fe(Mes)_2} + 4\ \mathrm{H(OAr)} + n\ \mathrm{LiN(TMS)_2} \longrightarrow \mathbf{Li_{\mathit{n}}Fe(OAr)_{2+\mathit{n}}} + 2\ \mathrm{H\text{-}Mes} + 2\ \mathrm{HN(TMS)_2}$$



Completed compounds are characterized with a variety of different equipment

<u>Molecular</u>

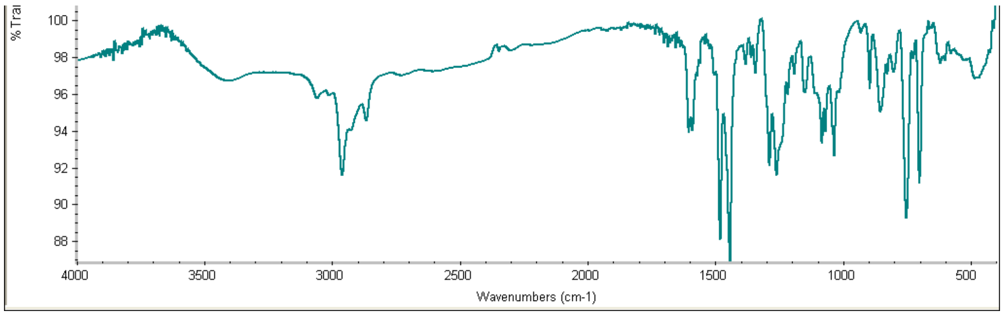
- FTIR
- Elemental Analysis
- Single Crystal XRD

<u>Material</u>

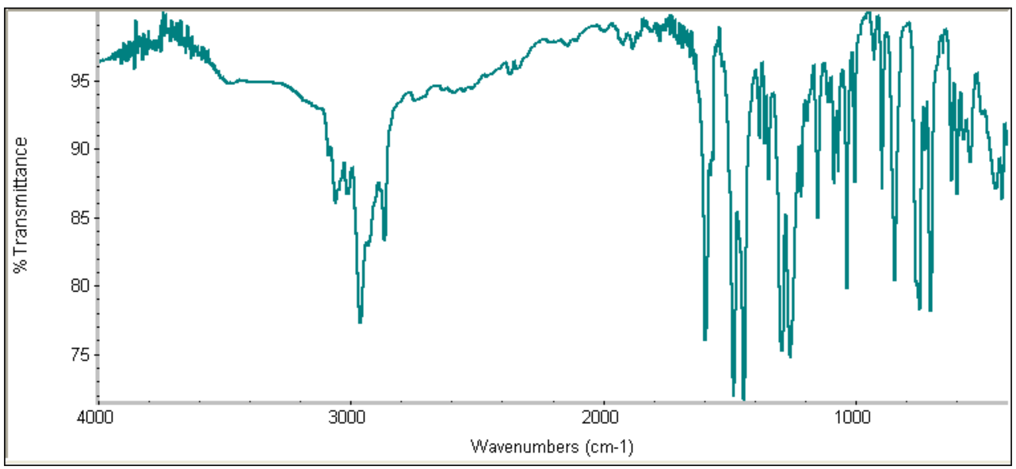
- TEM
- SEM
- Powder XRD

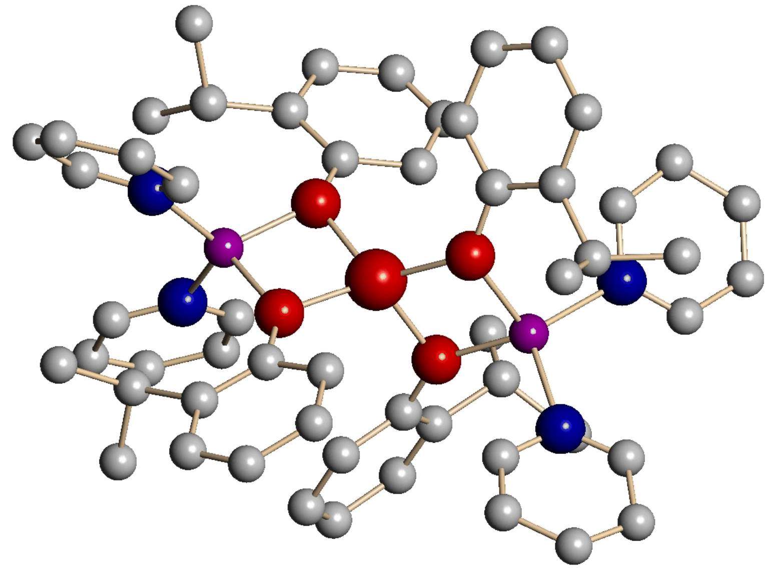
$\mathbf{Fe(Mes)_2} + 2\ LiN(TMS)_2 + 4\ H(\mathit{o}PP) \longrightarrow$

$Fe(oPP)_2(py)_3$



$FeLi_2(\mu\text{-}oPP)_4(py)_4$



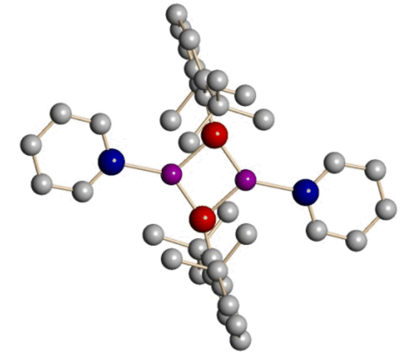


$FeLi_2(\mu\text{-}oPP)_4(py)_4$

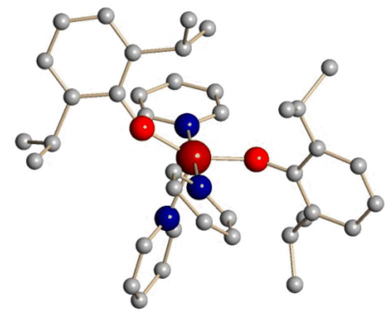
EA	Nitrogen	Hydrogen	Carbon
Theoretical	6.045%	6.950%	72.568%
Actual	6.0%	7.15%	72.86%

Coordination chemistry of $LiFe(OR)_x$ system is being elucidated.

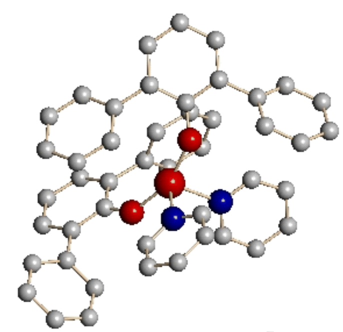
OAr	Tol	Py
OMP	$FeLi_2(OMP)_4$	$FeLi_2(oMP)_4$
OPP	$FeLi_2\ (OPP)_4$	$FeLi_2\ (oPP)_4$
OBP	$FeLi_2(OBP)_4$	$FeLi_2(OBP)_4$
DMP	$FeLi_2(DMP)_4$	$FeLi_2(DMP)_4$
DIP	$FeLi_2(DIP)_4$	$FeLi_2(DIP)_4$
DBP	$FeLi_2(DBP)_4$	$FeLi_2(DBP)_4$
DPhP	$FeLi_2(DPhP)_4$	$FeLi_2(DPhP)_4$

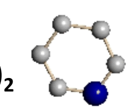


$Li_2(\mu\text{-DBP})_2(py)_2$

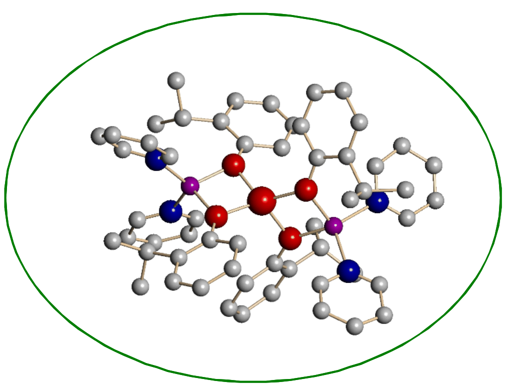


$Fe(DIP)_2(py)_3$

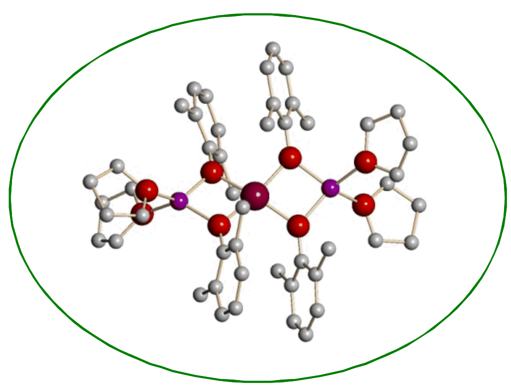




$Fe(DPhP)_2(py)_2$



$FeLi_2(\mu\text{-oPP})_4(py)_4$



$FeLi_2(\mu\text{-DMP})_4(THF)_4$

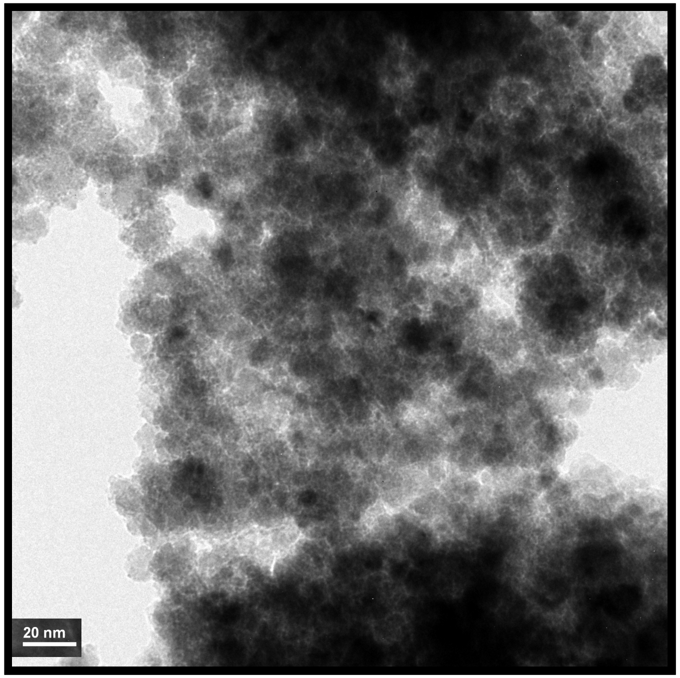
A Solvothermal Route was taken in development of the $FeLi_2O_4$ nanomaterials

Solvothermal Route

$Li_2Fe(OAr)_4 \rightarrow LiFe_2O_4$

Parr Digestion Bomb

$Li_2Fe(oPP)_4 \rightarrow LiFe_2O_4$



PXRD

Summary and Conclusion

- Synthesize SSP's
- Develop Nanomaterials
- Characterize Compounds
- Test utility as Li-Ion battery cathode material