

# Student Involvement in Scientific Research

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Department of Physics



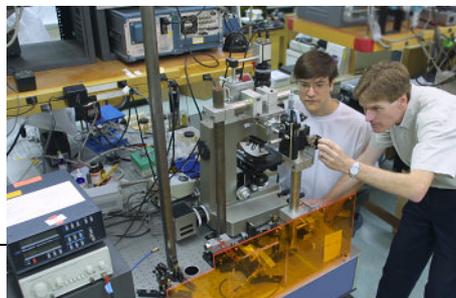
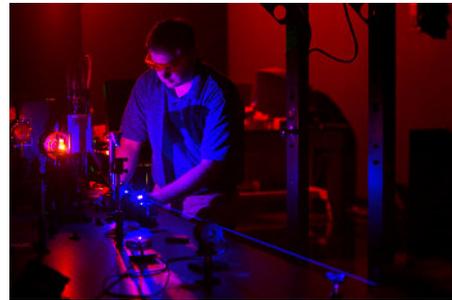
WAKE FOREST  
UNIVERSITY

Sept. 5 & 12, 2012

General comments:

- Important component of your education; in addition to studying science through classwork, provides a **first-hand experience of the scientific method**

For example, picture yourself here:



...

## How to choose a research group:

- Pick subject area that interests you – biophysics, condensed matter physics, gravitational/astro physics
  - Decide whether you prefer theoretical/computational or experimental physics
  - Talk to several faculty to help you decide what fits you best
  - It is possible to work with several groups during your tenure at WFU; stick with one group at least one year
  - Decide whether you prefer to work with a large group or a small group
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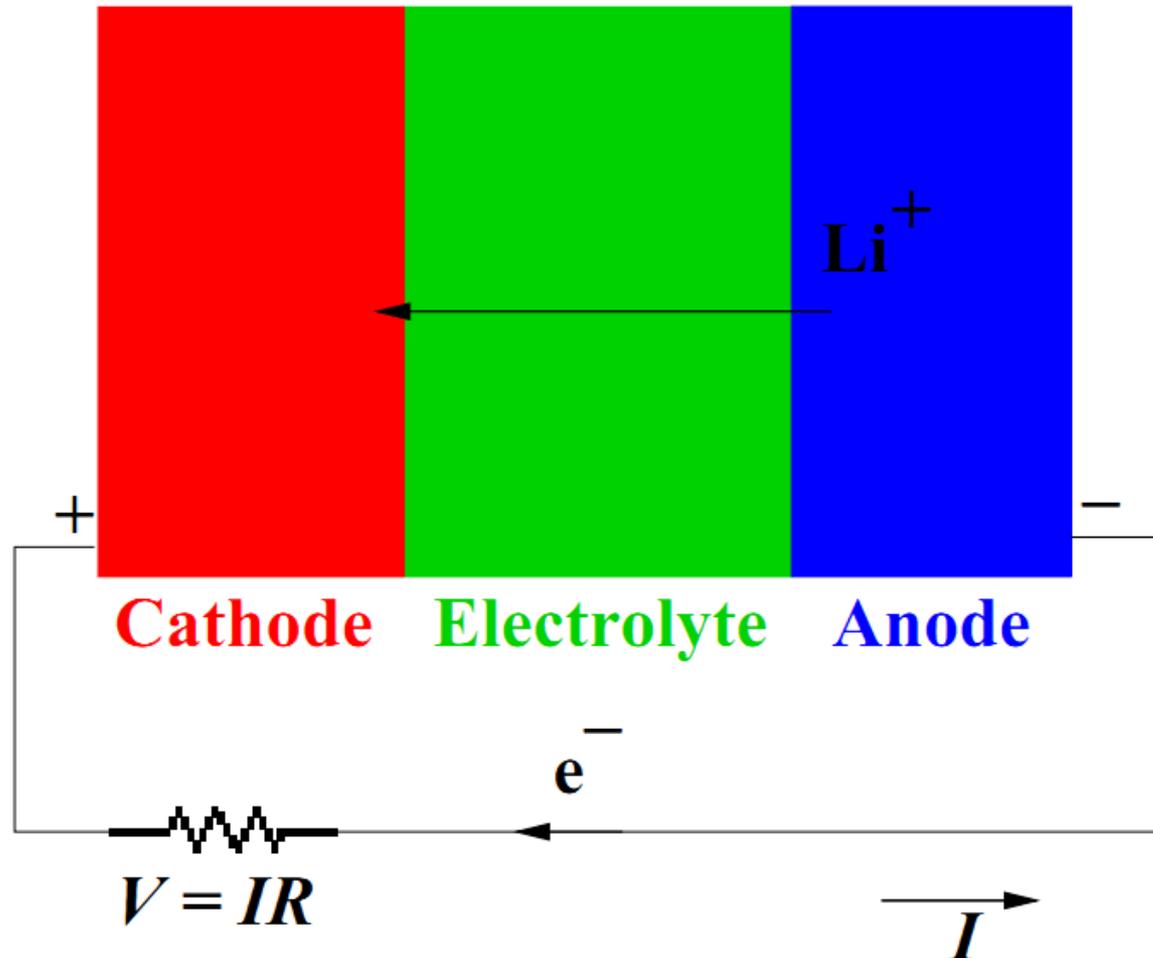
Pitch talk:

## The THRILL and EXCITEMENT of Computational Materials Research

Focus:

- Predict and understand materials and their properties
  - Use and develop computational tools for materials research
  - Emphasis on earth-abundant and environmentally-friendly materials for rechargeable batteries
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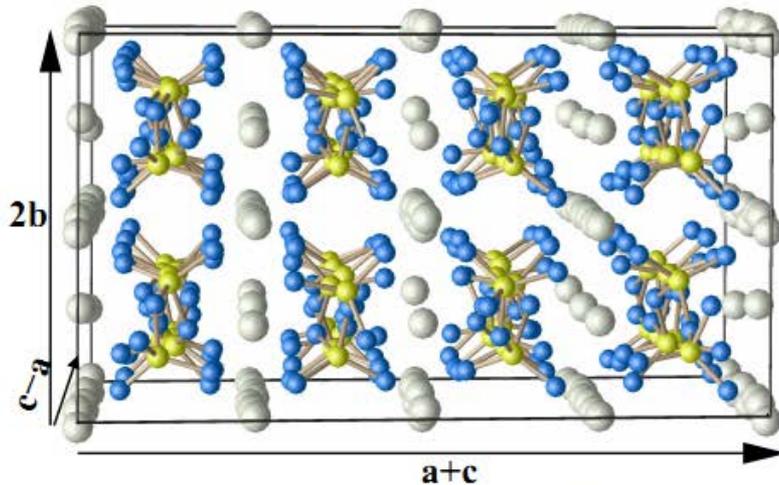
# Materials components of a Li ion battery



## Phosphate chain materials: $\text{LiPO}_3$ plus N

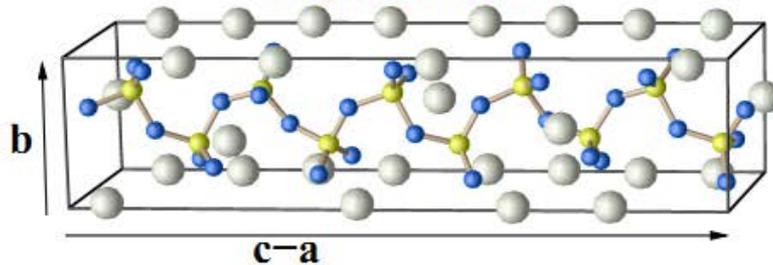
$\text{LiPO}_3$  in  $P2/c$  structure; 100 atom unit cell

Chain direction perpendicular to plane of diagram



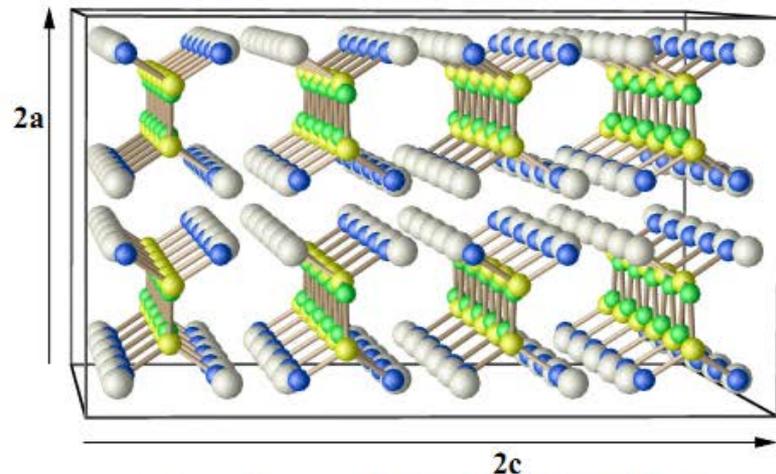
Ball colors:  $\bullet$  = Li,  $\bullet$  = P,  $\bullet$  = O.

Single chain view



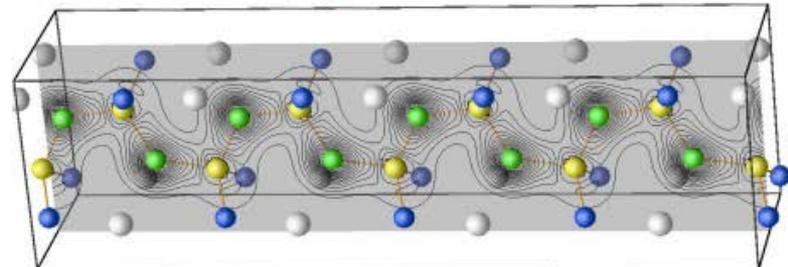
$s_1\text{-Li}_2\text{PO}_2\text{N}$  in  $Pbcm$  structure; 24 atom unit cell

Chain direction perpendicular to plane of diagram



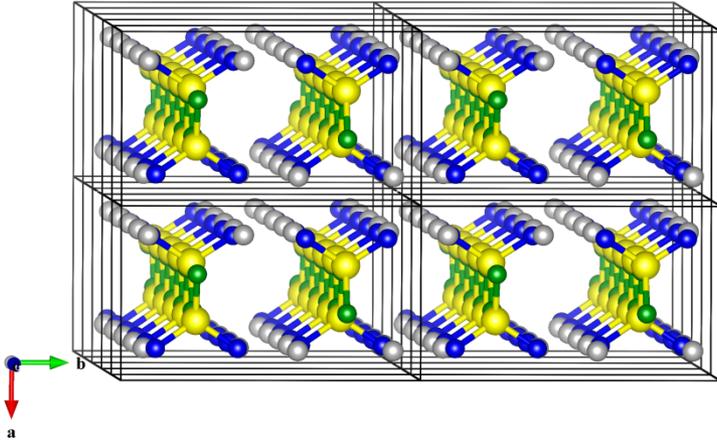
Ball colors:  $\bullet$  = Li,  $\bullet$  = P,  $\bullet$  = O,  $\bullet$  = N.

Single chain view

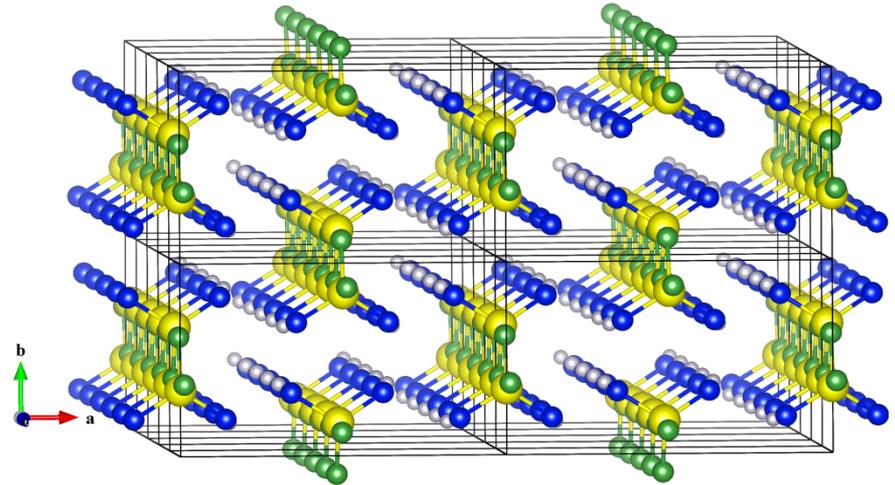




Du-Holzwarth structure,  
predicted (2010)



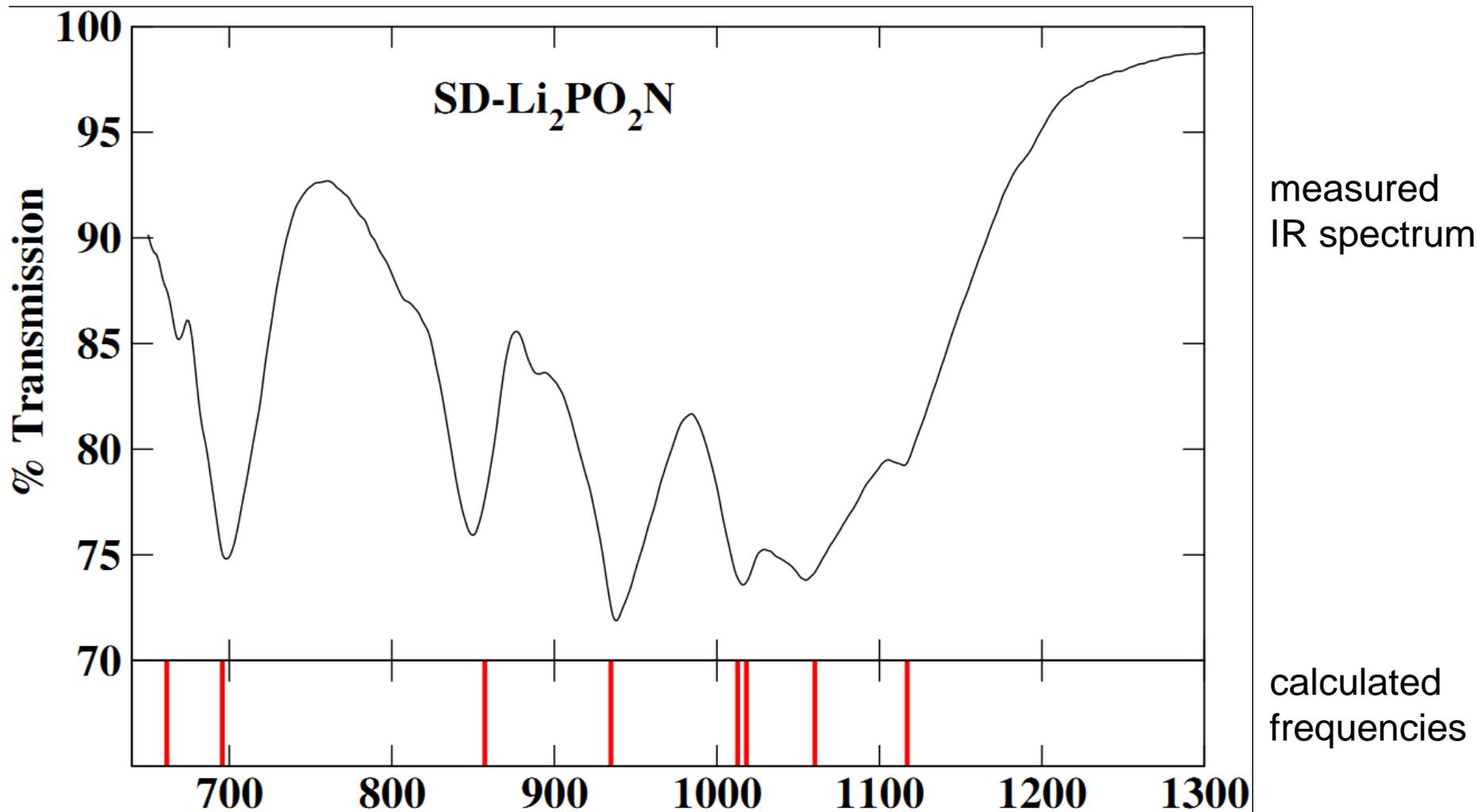
Seneviranthe\*-Day\*\* structure,  
synthesized, analyzed (2012)



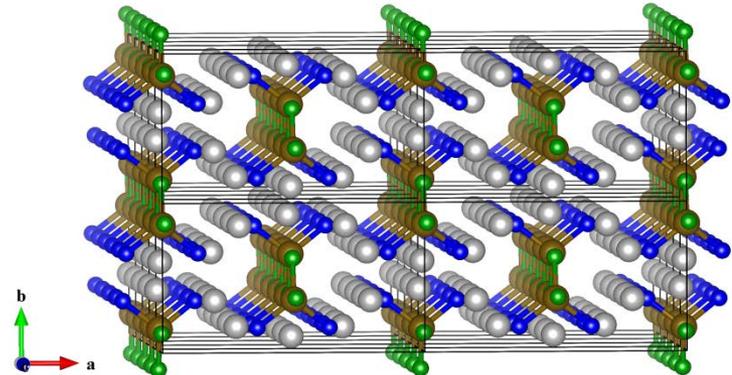
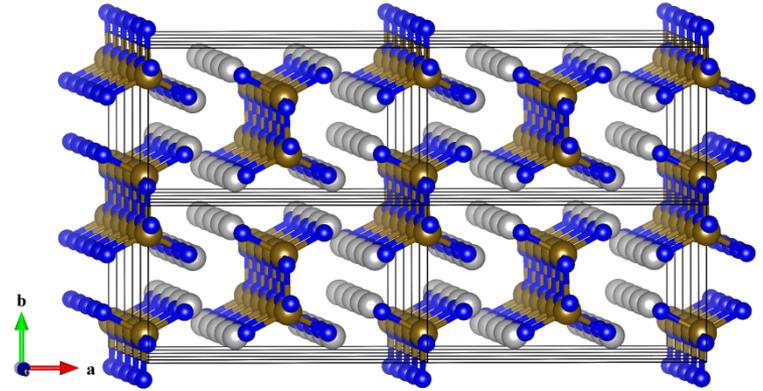
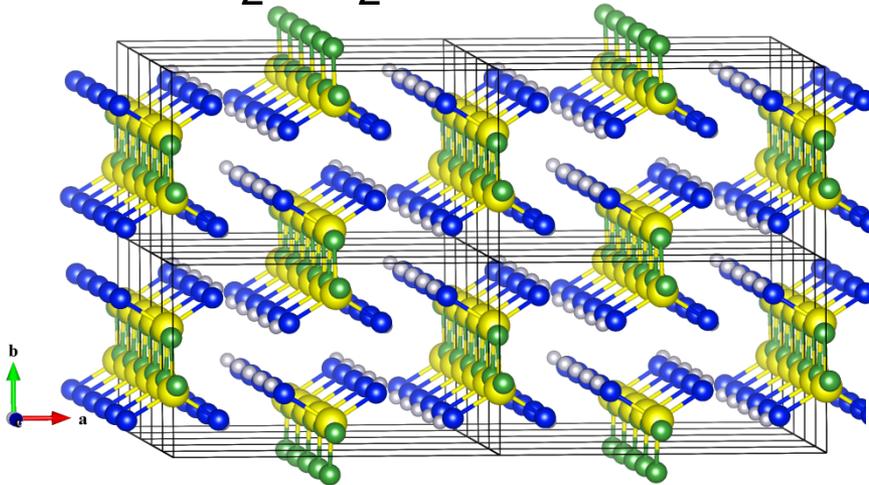
$$E_{\text{SD}} - E_{\text{s2}} = -0.1 \text{ eV/fu}$$

\*CEES fellow

\*\*X-ray crystallographer



Other possible electrolyte materials



## Requirements for computational materials research

- Interest in materials and in computation  
(can jump in at various levels)
- Patience and willingness to learn

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