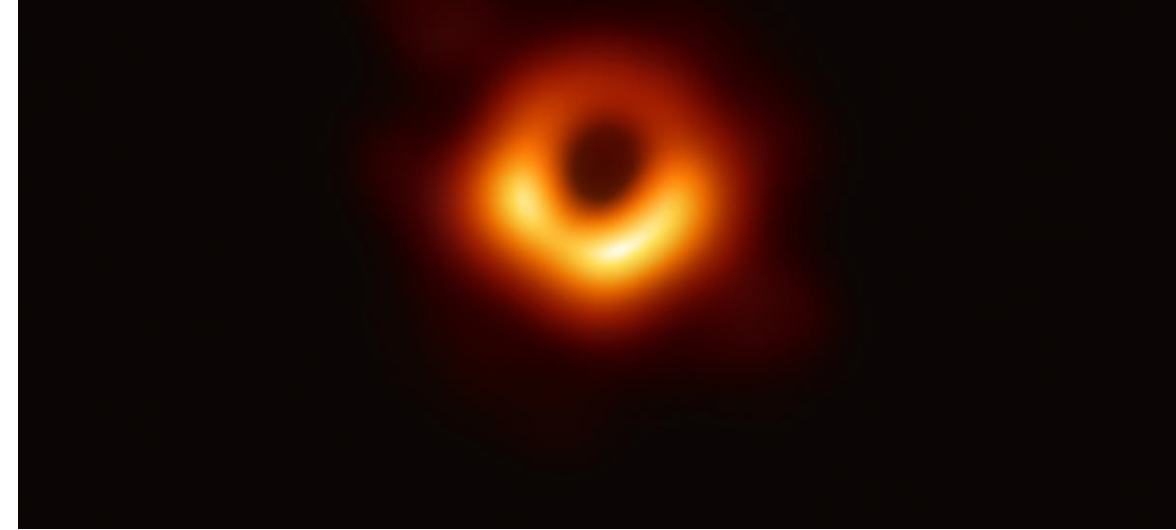# Diffpy-CMI,

Rob Koch
Brookhaven Lab

Outline

- Python? No silly walks here…
- Diffpy-CMI
- Beating a dead horse: fitting Nickel
- Dead horse reprise: Nanocrystals
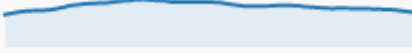- Some physics: the case of $SrFe_2As_2$

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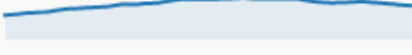
Python? No silly walks here…

- Why use python?
  - It's free!
  - It's easy!
  - It's open source!
  - It's fast!*

*if you do things properly

- How can I use python?
- First, install it:
  - https://www.anaconda.com/distribution/ (Windows)
  - https://docs.conda.io/en/latest/miniconda.html (Unix)
- Next, apply it to your problems:
  - Read, plot your data (run away from MS Excel…)
  - Manipulate your data
  - Google

https://youtu.be/BIvezCVcsYs

Rank	Language	Monthly Active Users	Trend
1	JavaScript	22.63%	
2	Python	14.75%	
3	Java	14.01%	
4	C++	8.45%	
5	C	6.03%	

https://www.benfrederickson.com/ranking-programming-languages-by-github-users/

For your sake and ours, please use python 3 (not 2)…

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Diffpy-CMI

- Why would I use it?
  - PDFgui will only get you so far
  - A prerequisite of all advanced modelling is initial basic understanding
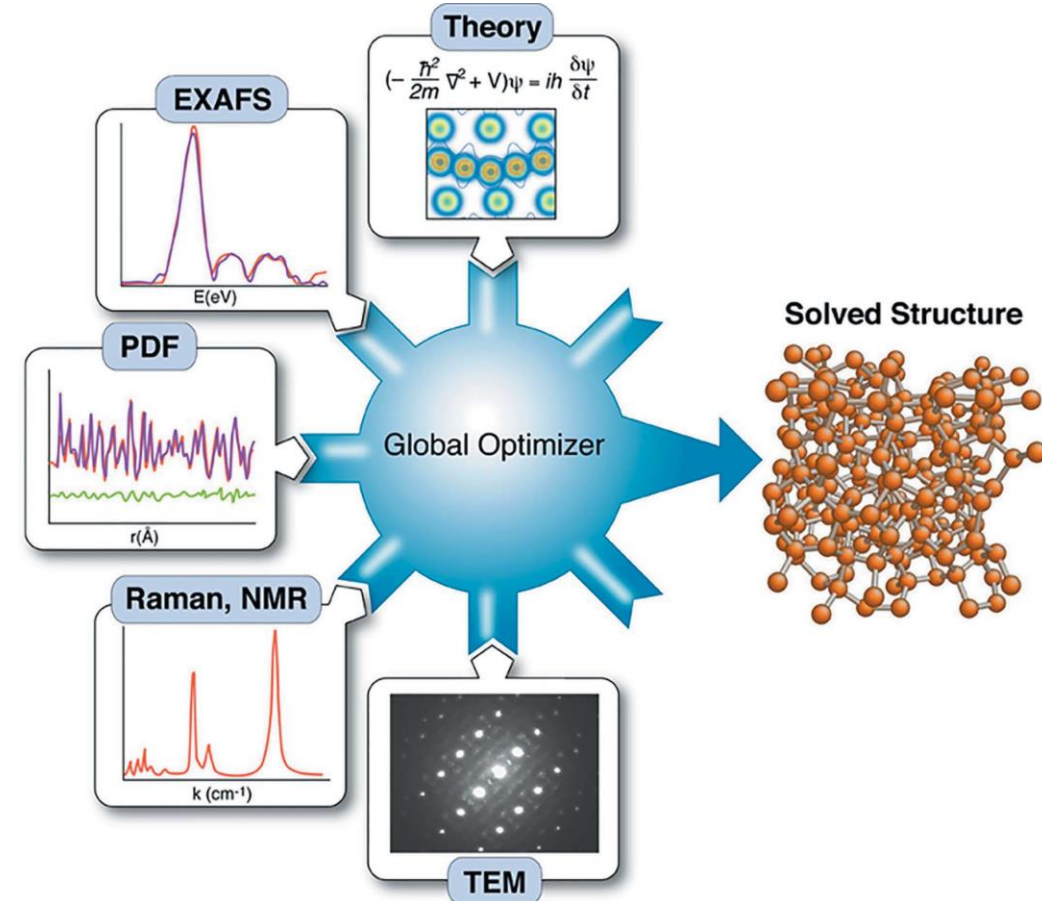 - Python can streamline the handling and post processing of many datasets

- Where can I get it?
  https://www.diffpy.org/products/diffpycmi/

- What if I need help?
  https://groups.google.com/forum/#!forum/diffpy-users
- What if I want to help? https://github.com/diffpy/

- What if I still need help? rkoch@bnl.gov
  - I can offer advice
  - I can help with minor debugging

  - I cannot reduce your data
  - I cannot write your code
  - I cannot give you CPU cycles

Juhas, P., Farrow, C., Yang, X., Knox, K. & Billinge, S. (2015). *Acta Cryst. A71*, 562-568. https://doi.org/10.1107/S2053273315014473

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Let's do some practical examples

- You can have the source code: https://github.com/rjkoch/2019_ORNL_total_scattering

- You can follow along: https://mybinder.org/v2/gh/rjkoch/2019_ORNL_total_scattering/master

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Beating a dead horse: fitting Nickel

- Let's look at our prototype easy example
  - Fit PDF of nickel standard to get instrument parameters

Dead horse reprise: Nanocrystals

- Let's fit a nanocrystalline platinum system
  - We use our instrument parameters we refined in example 1

Some physics: the case of $SrFe_2As_2$

- Iron-based superconductor
- Phase transition (tetragonal to orthorhombic) at about 200 K
- Some distortions persist….
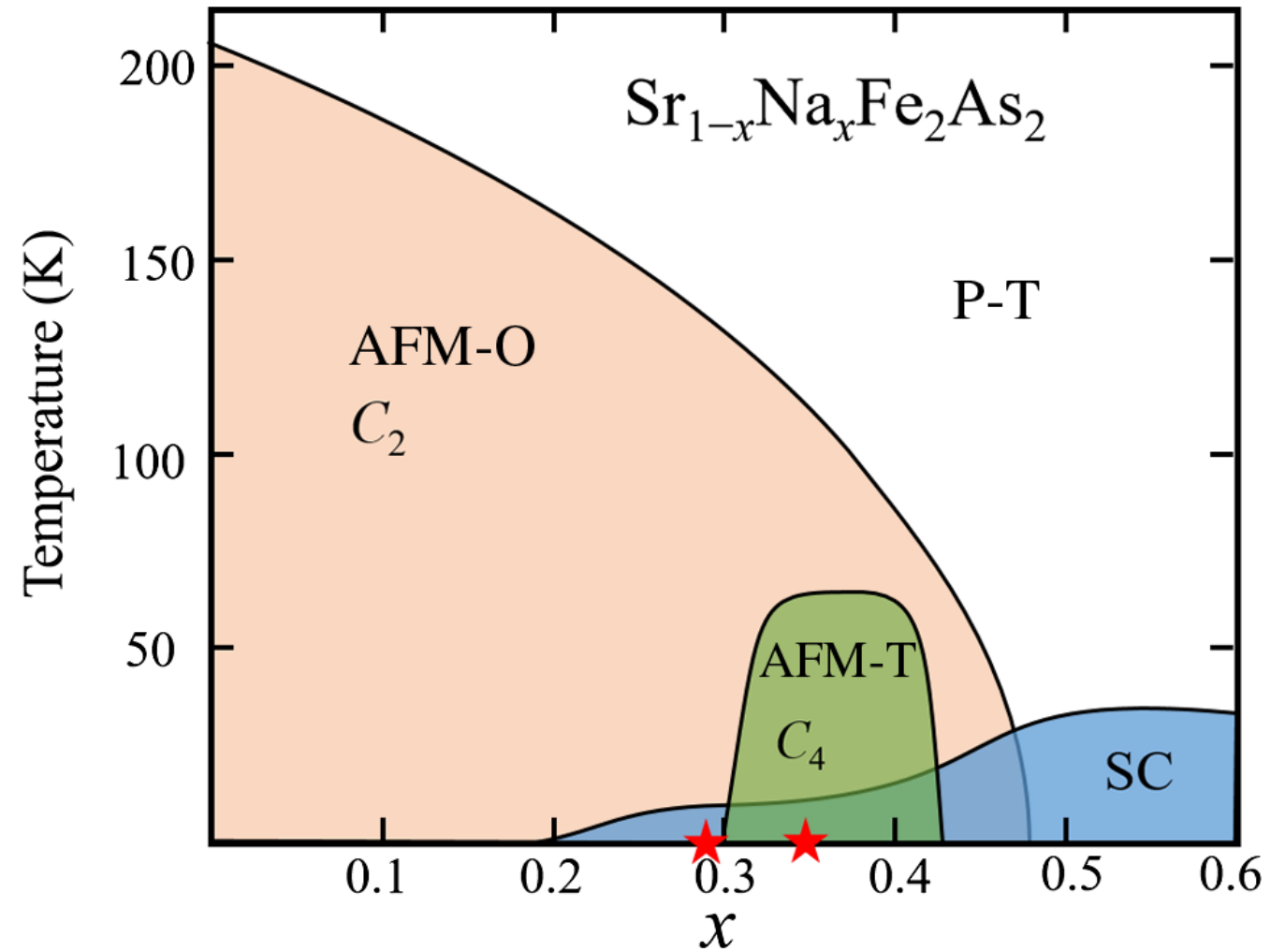
B. A. Frandsen *et al. Phys. Rev. Lett*. **119**, 187001 2017
https://doi.org/10.1103/PhysRevLett.119.187001

25 Oct 2019