Applications of principal component analysis to pair distribution function

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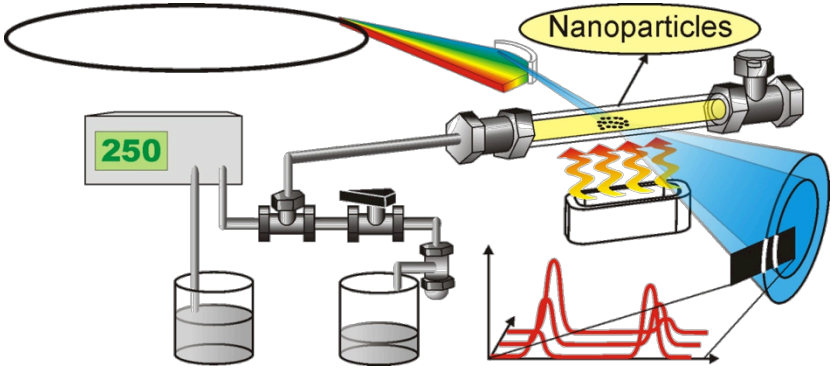
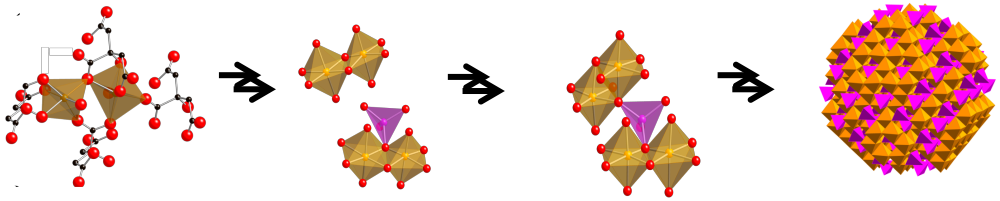


Why do we do pair distribution function analysis



How does we use PCA on pair distribution function data?

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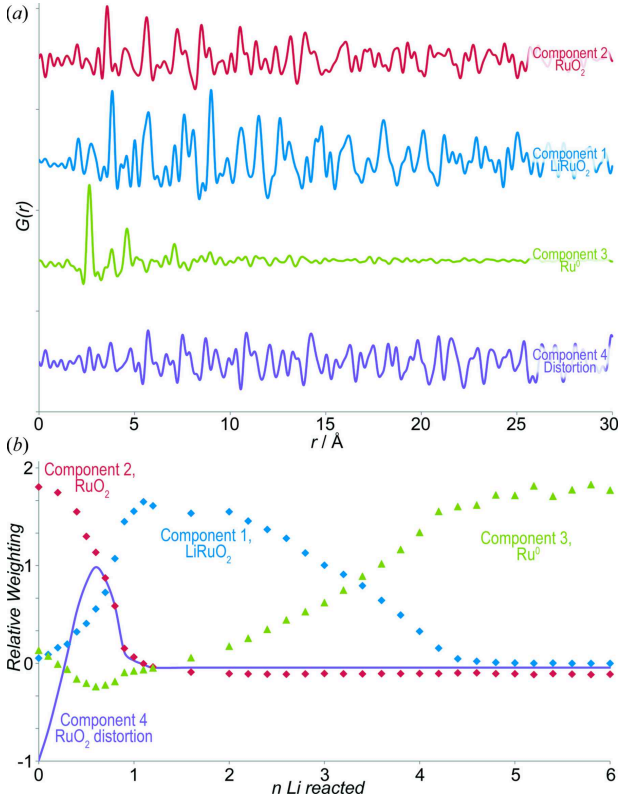
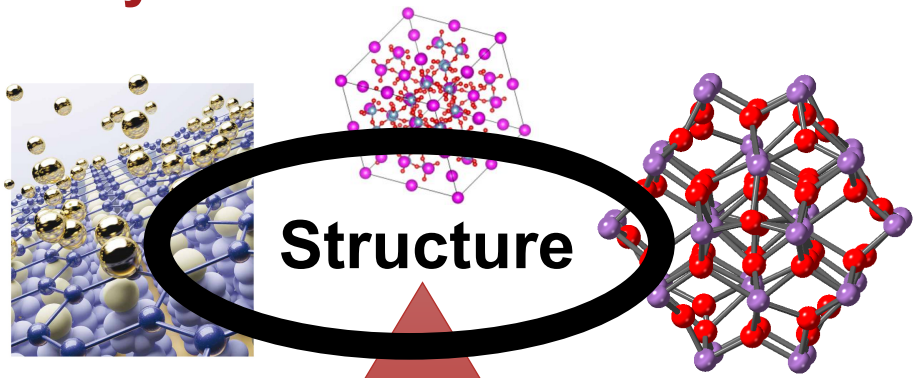
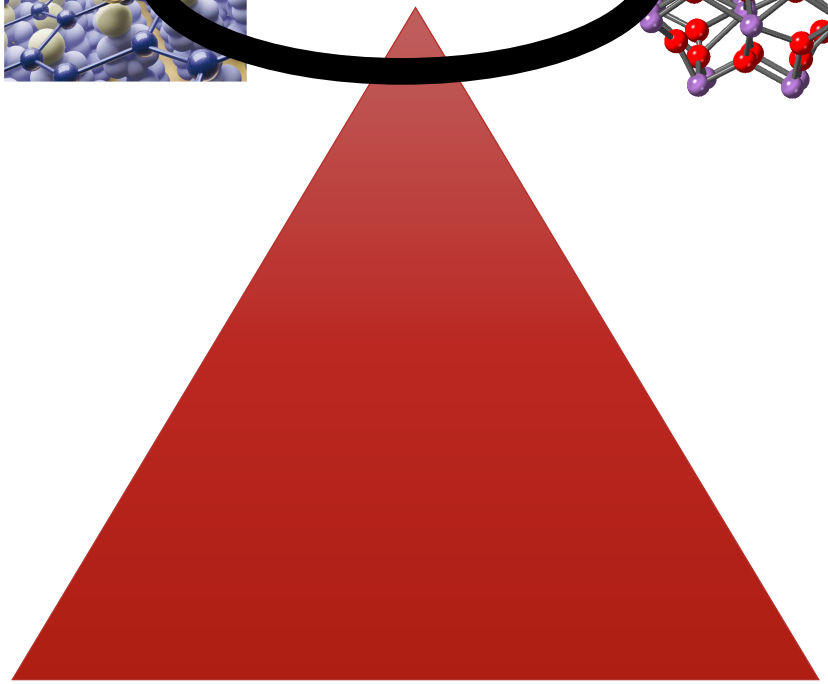
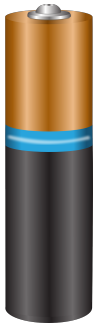


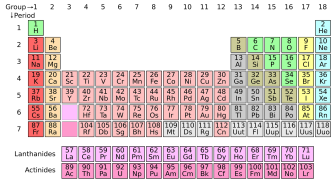
What is principal component analysis

The Holy Grail of Materials Chemistry



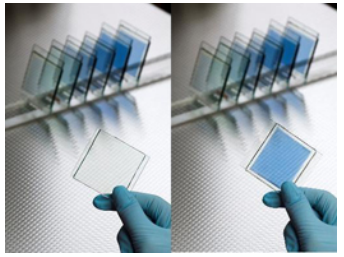




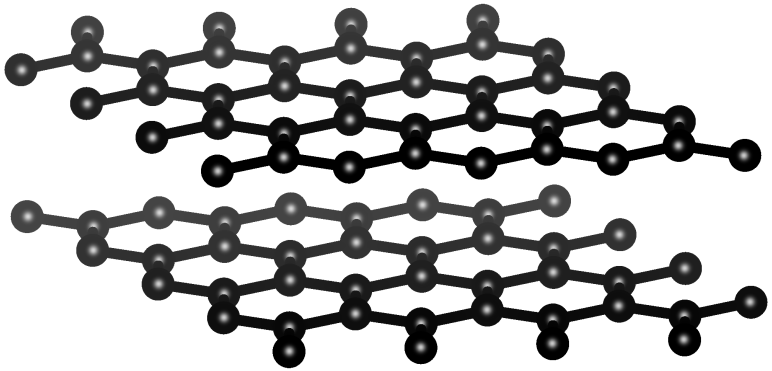


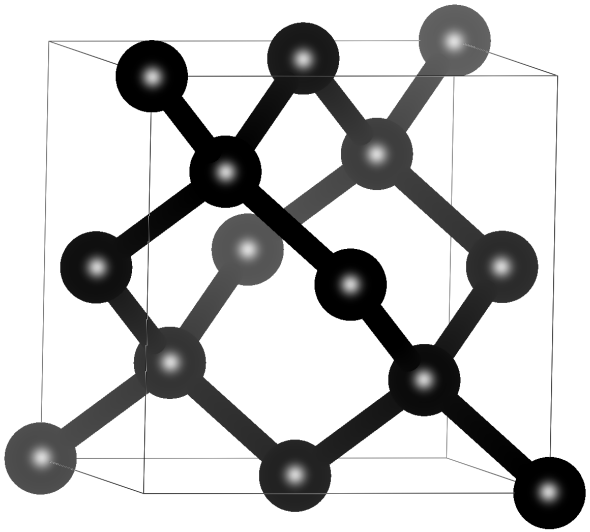
Synthesis

Properties



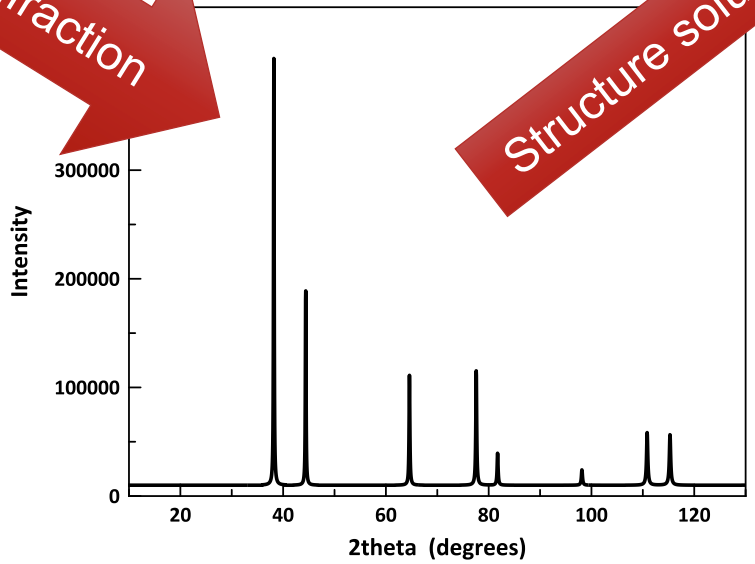
Properties and structure are directly connected



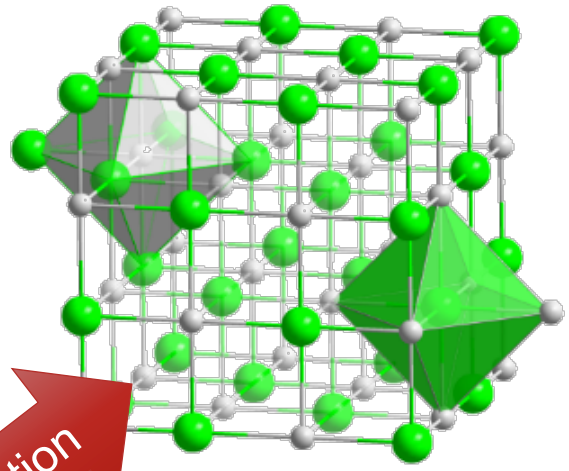


X-ray diffraction from bulk materials

X-ray diffraction



Structure solution



Constructive interference due to periodicity

New possibilities with 3rd generation synchrotron and high energy neutron facilities

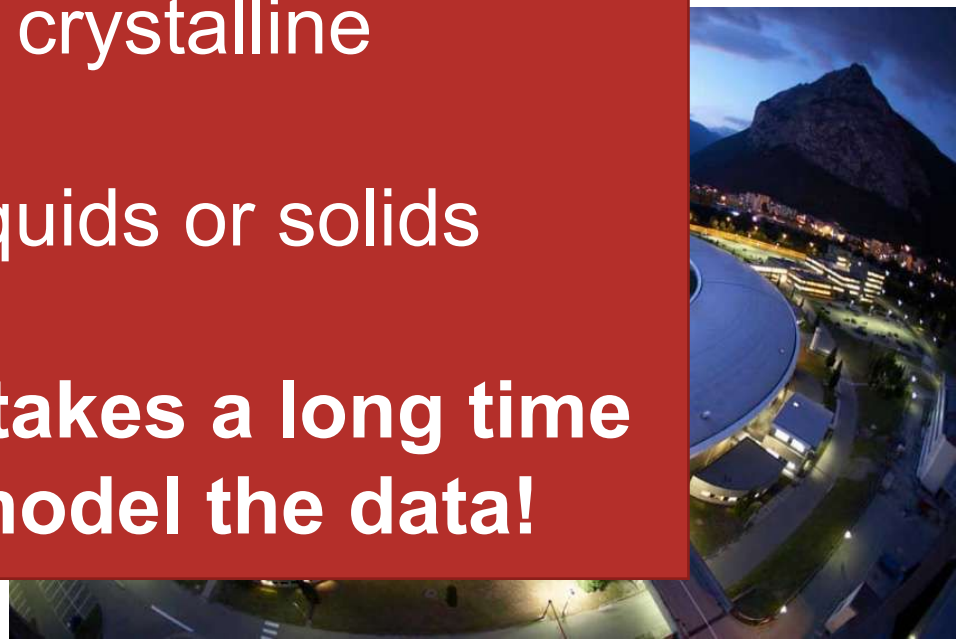
- **High energy**
- **High X-ray flux!**
- **More signal!**
- **Lots of data!**

All classes of materials

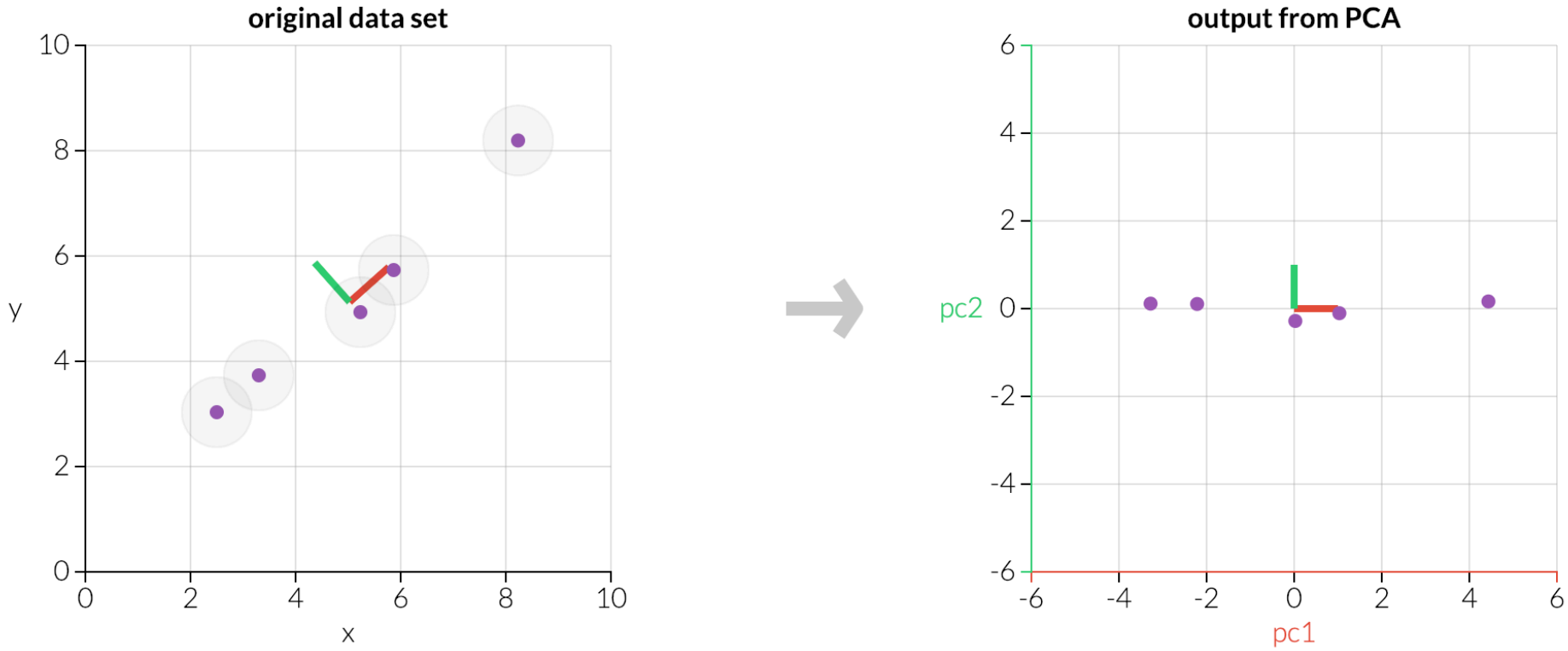
Amorphous, nanostructured and crystalline

Liquids or solids

But it takes a long time to model the data!



Principal Component Analysis in 2 dimensions

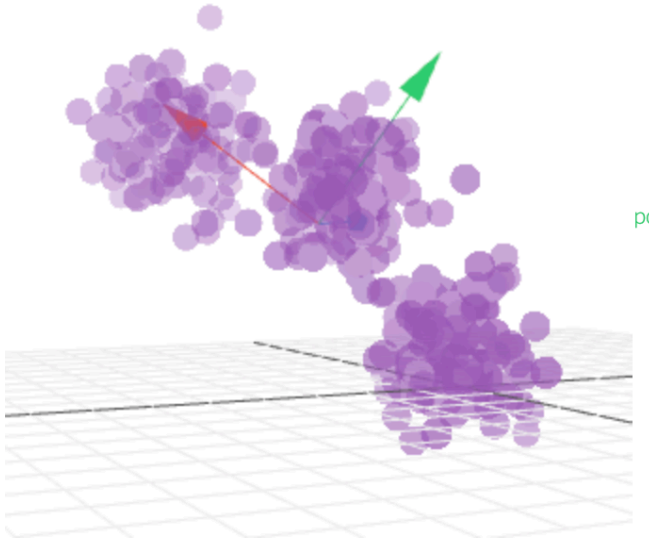


- **2 linear regressions**
- **Scaling – difficulties with chemical systems??**
- **Information in the PC's**

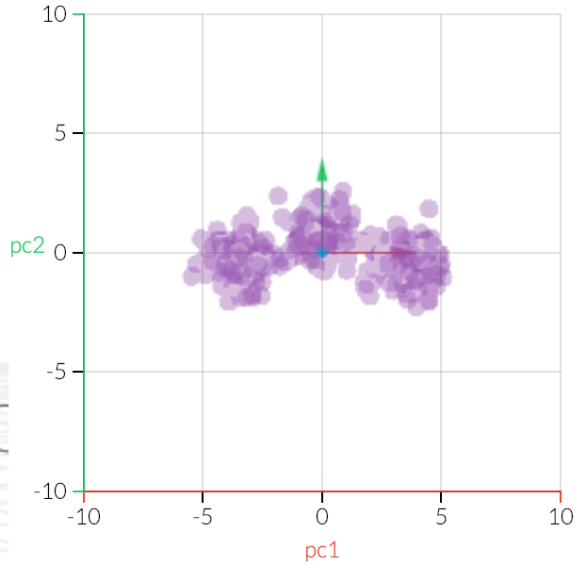
http://setosa.io/ev/principal-component-analysis/

Principal Component Analysis in 3 dimensions

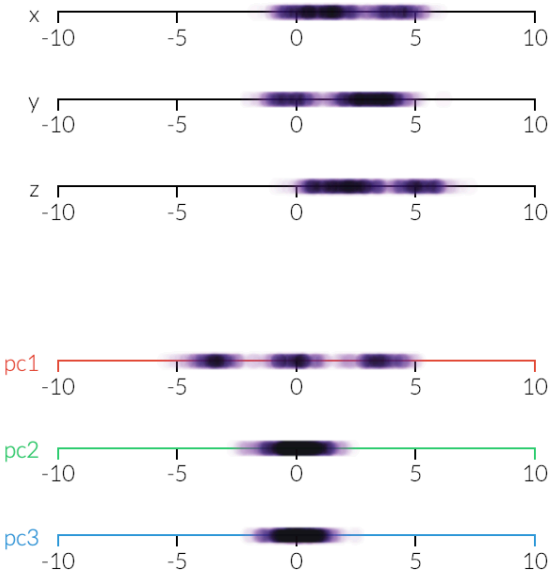
- **3D visualization**



Projected to 2D



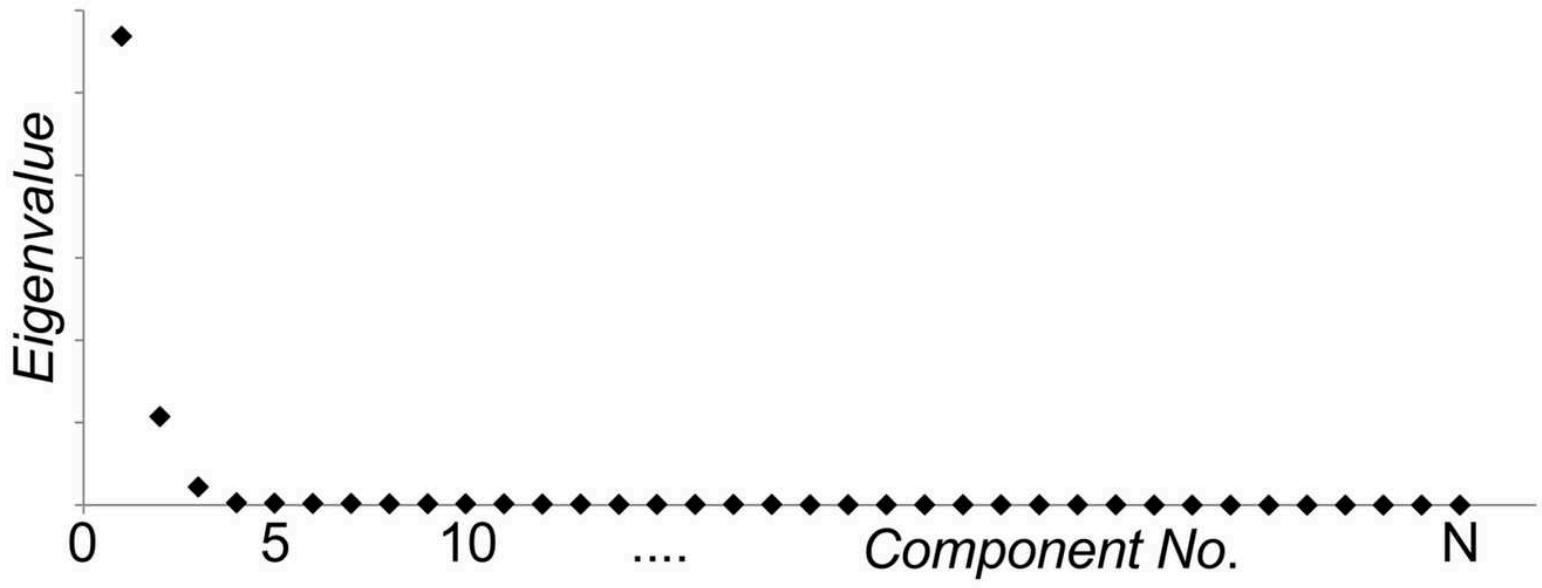
Projected to 1D



- **3 linear regressions**
- **Difficult to visualize multiple dimensions**
- **Clustering**
- **Robustness with pair distribution function data**

http://setosa.io/ev/principal-component-analysis/

PCA Scree plot



- **How many PC's describes the data?**
- **How much information in the PC?**

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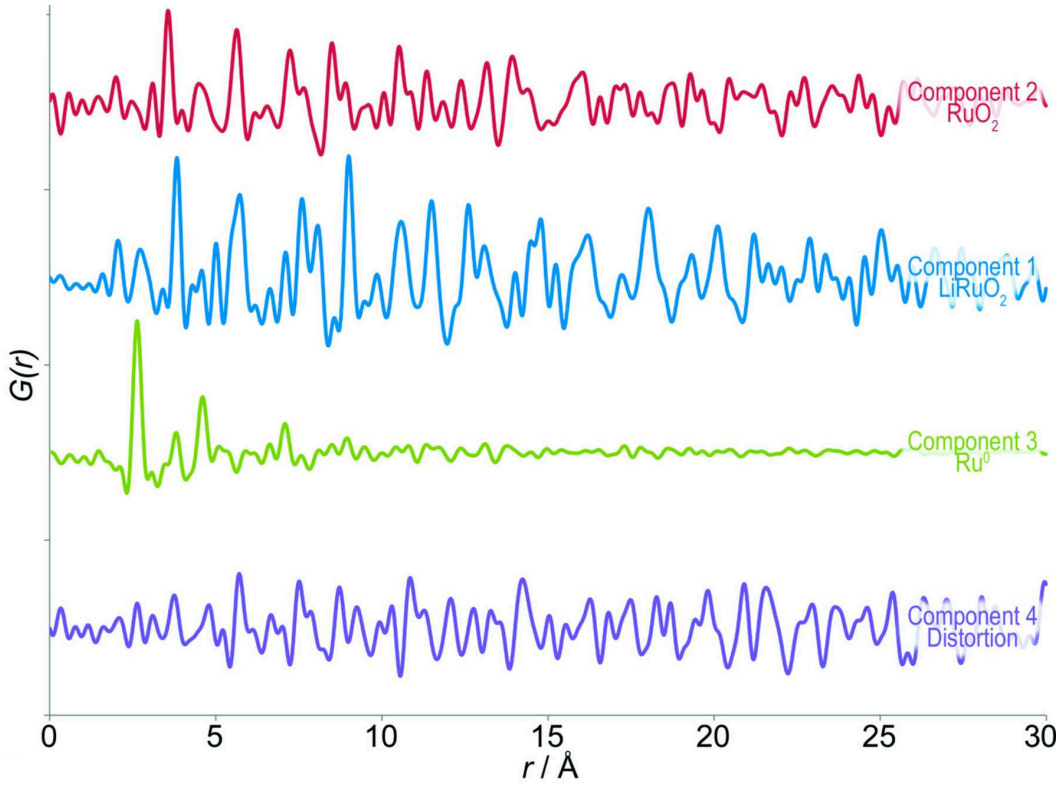
Principal Components plot



- How does the PC look like?
- Are they physical?
- Does a structure relate to 1 or multiple PC's?

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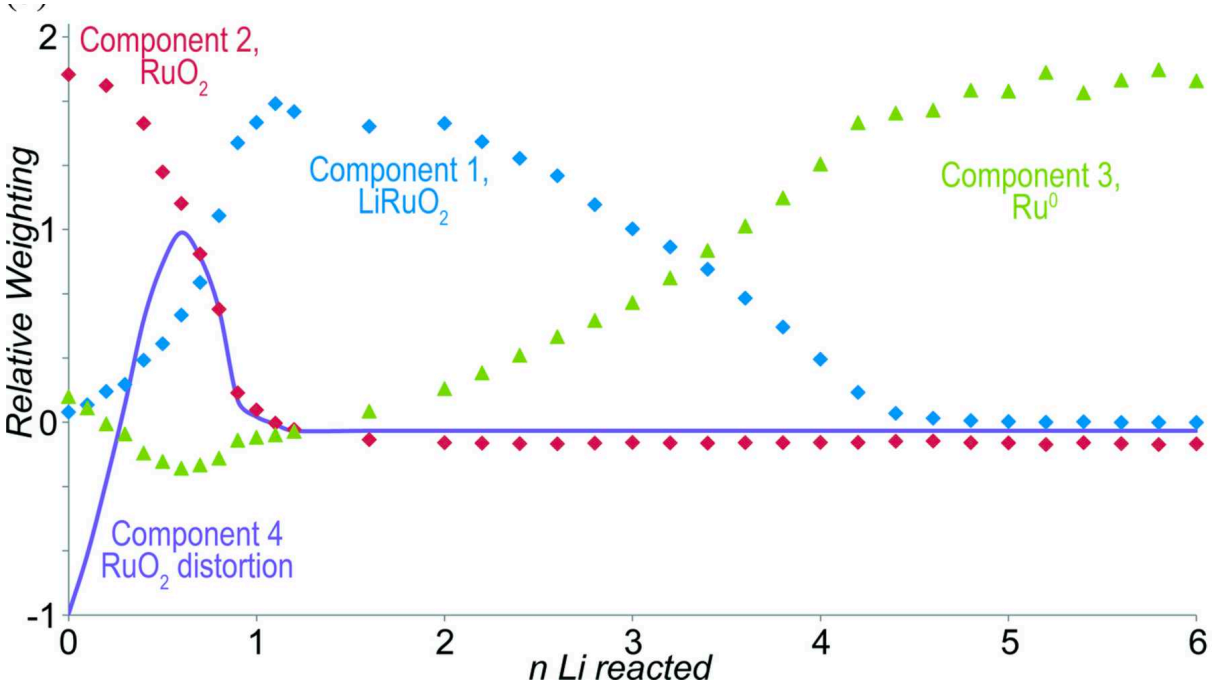
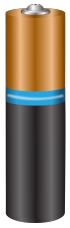
Ratio of Principal Components



- **How does the ratio of PC's change during the reaction?**



RuO_2 → Li_xRuO_2 → Ru + Li_2O

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Conclusion:
Principal component analysis to pair distribution function

- **Modelling of PDF data by conventional techniques are time-consuming.**
- **PCA on pair distribution function data is fast.**
- **PCA does not need any prior knowledge (bias) of the chemical structure.**
- **PCA can identify trends that the human eye cannot – peak overlap, large amounts of data, complicated changes.**
- **This article shows that PCA is efficient in modelling pair distribution function data.**