Understanding angle-resolved photoemission data in space and time

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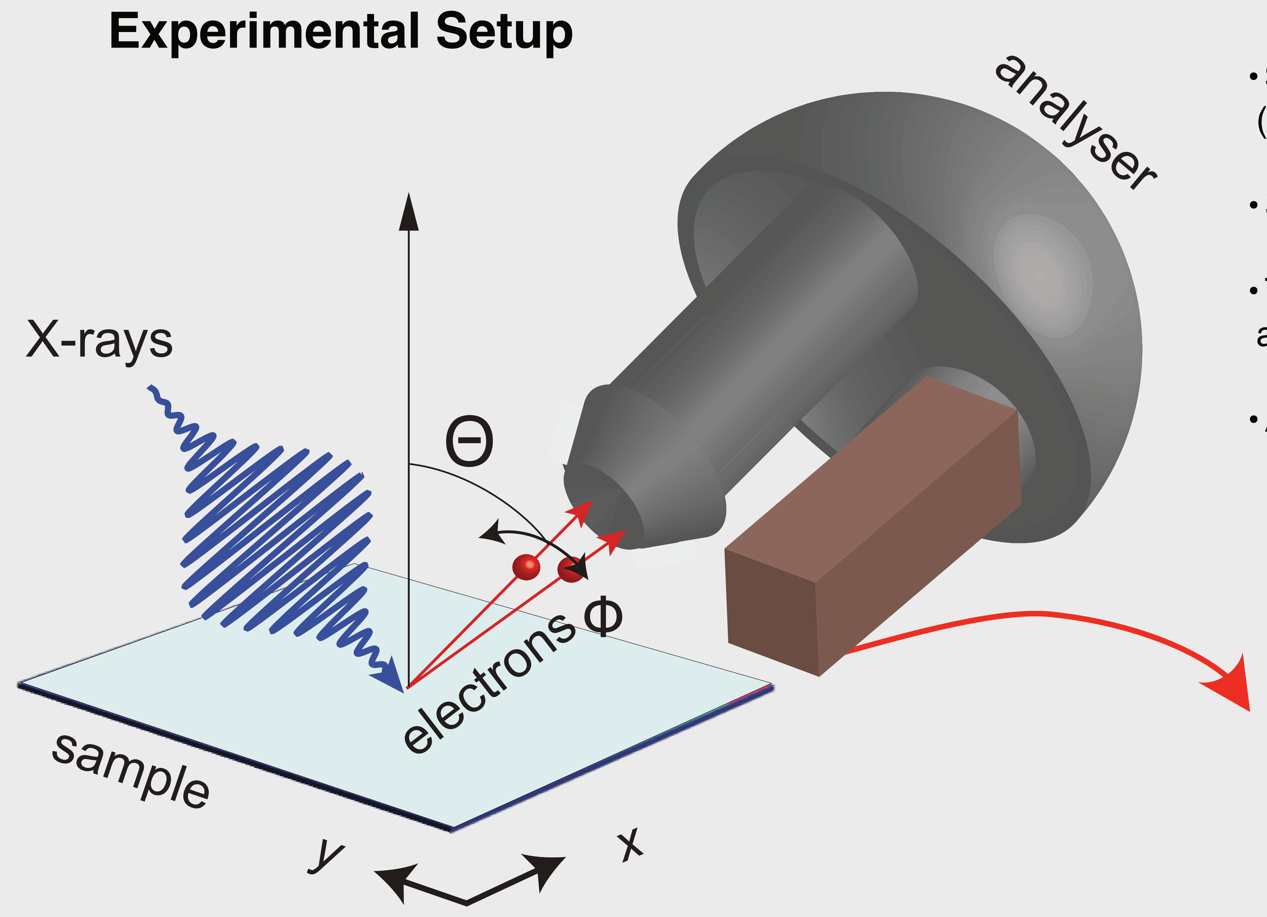
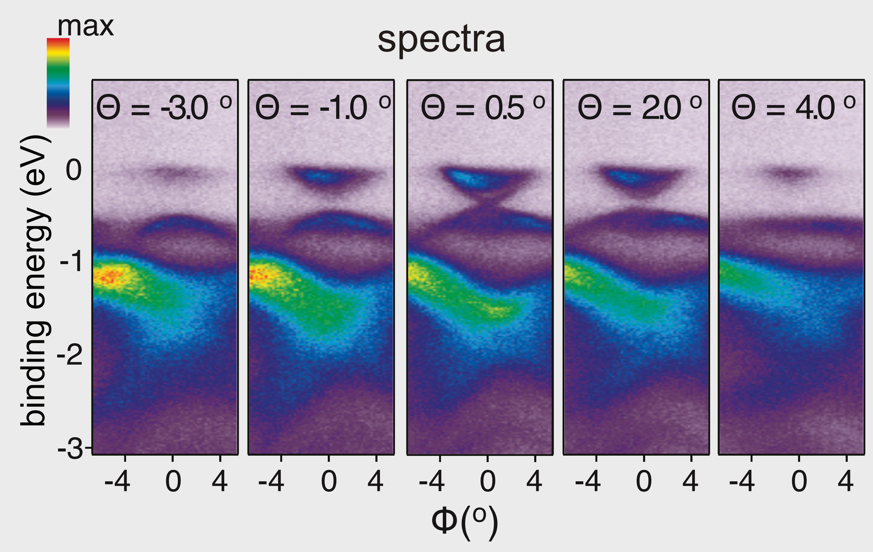
Introduction

- **Angle-resolved photoemission spectroscopy (ARPES)** is an experimental technique to determine the electronic structure of quantum materials. It is based on the photoelectric effect.
- **MicroARPES** adds spatial resolution to study inhomogeneous samples, operating electronic devices, phase separation and phase transitions.
- **Time-resolved ARPES** adds time resolution, opening a window on dynamic processes, such as coherent phonons, the melting of charge density waves or light-induced transient states of matter.
- Both approaches increase the number of parameters that can be / need to be explored and the complexity of the data.
- Clustering techniques, partially combined with autoencoder networks, can help to uncover trends in a complex multi-dimensional parameter space.

Experimental Setup

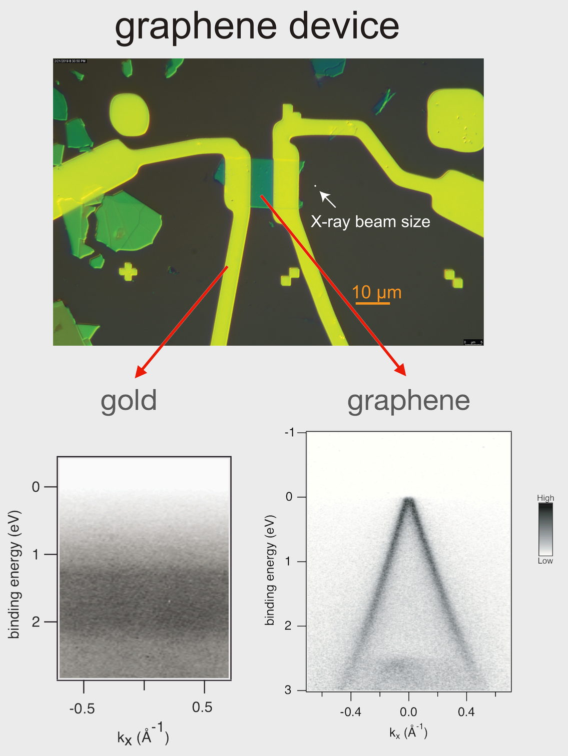


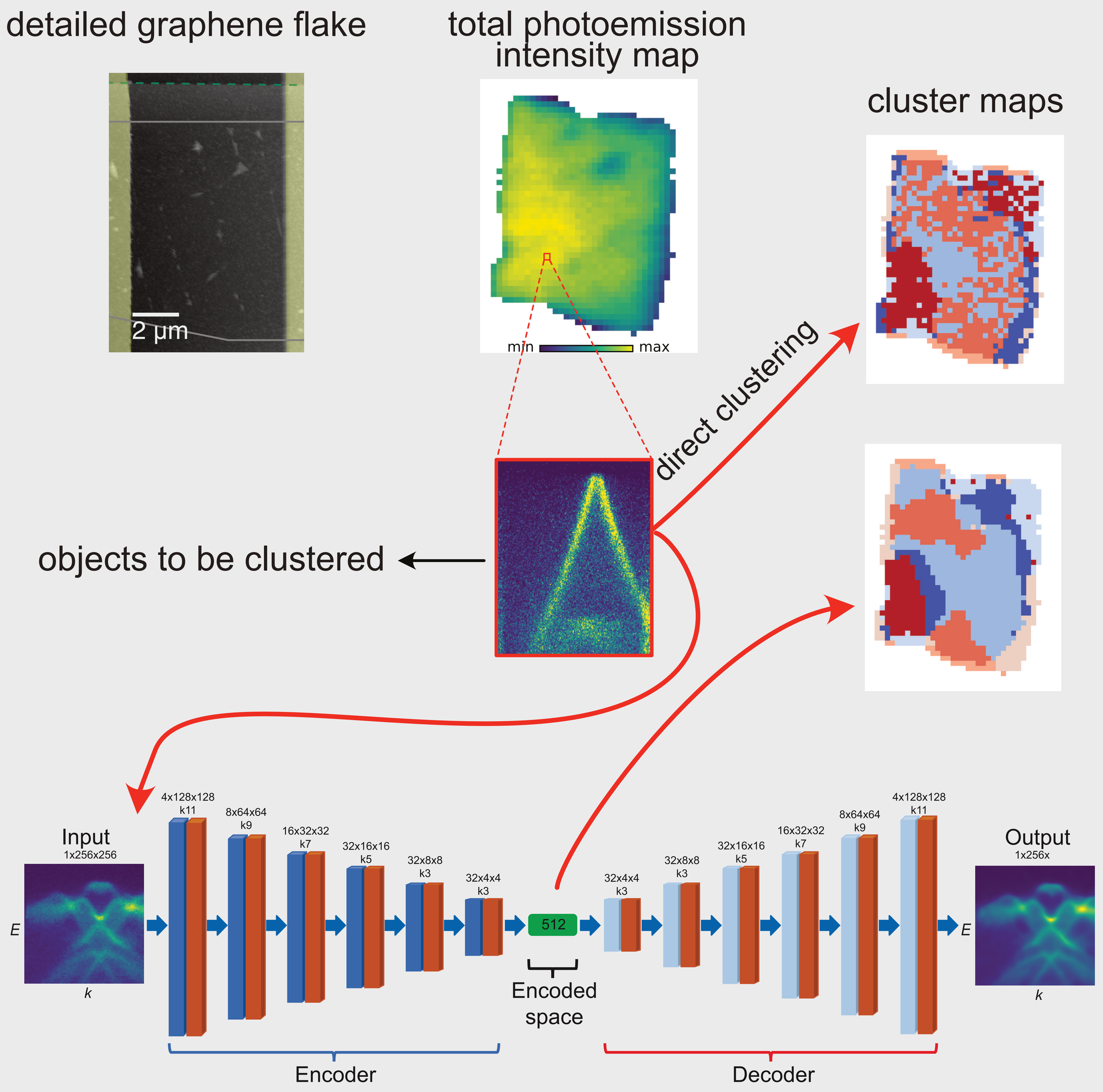
- **Spectra** are the photoemission intensity as a function of energy (vertical scale) and a single emission angle Φ (horizontal scale).
- Spectra can be viewed as "picture" of the band structure.
- The entire angular space can be explored by changing the other angle (Θ).
- Angles can be converted to crystal momentum (k_x and k_y).



MicroARPES

- X-ray beam is tightly focused and moved across the sample, turning ARPES into a microscopic technique.
- Permits study of inhomogeneous materials, electronic devices, phase separation, phase transitions.
- More experimental parameters: energy, two emission angles, position on the sample (x, y).
- Objects to be clustered: 2D spectra.
- Used to identify relevant / interesting areas.





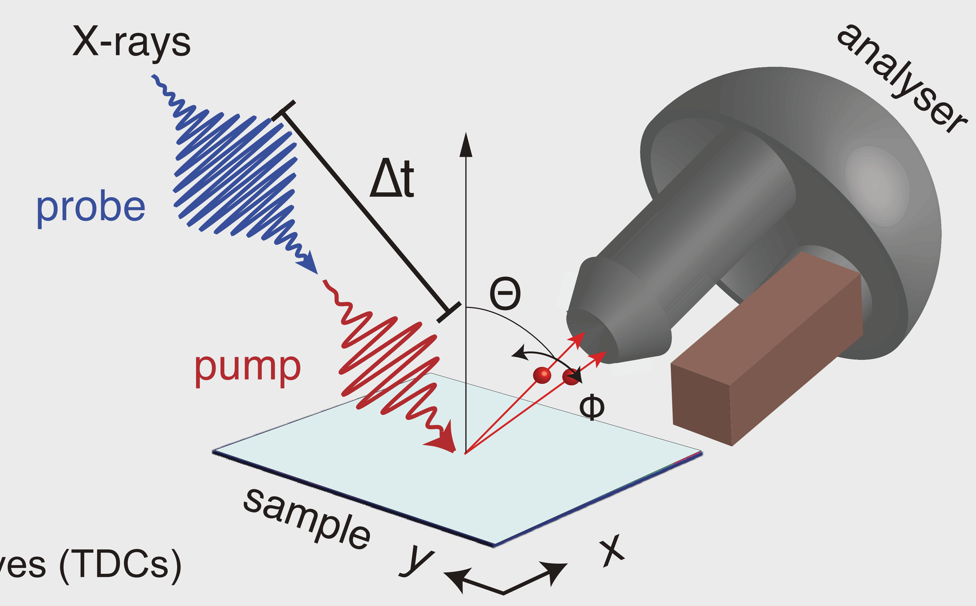
Conclusions

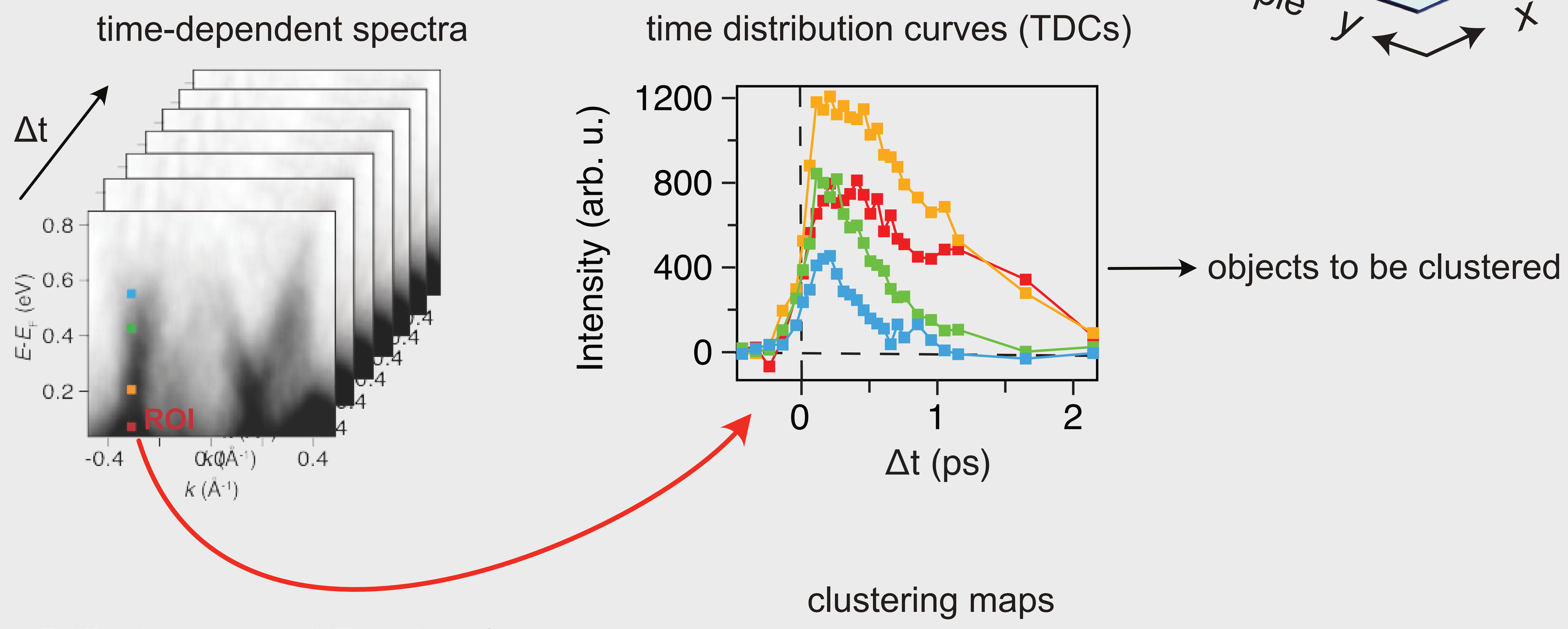
- k-means is excellent to find structure in microARPES data.
- No (biased) fitting model required.
- A well-trained autoencoder improves both speed and quality of the clustering.

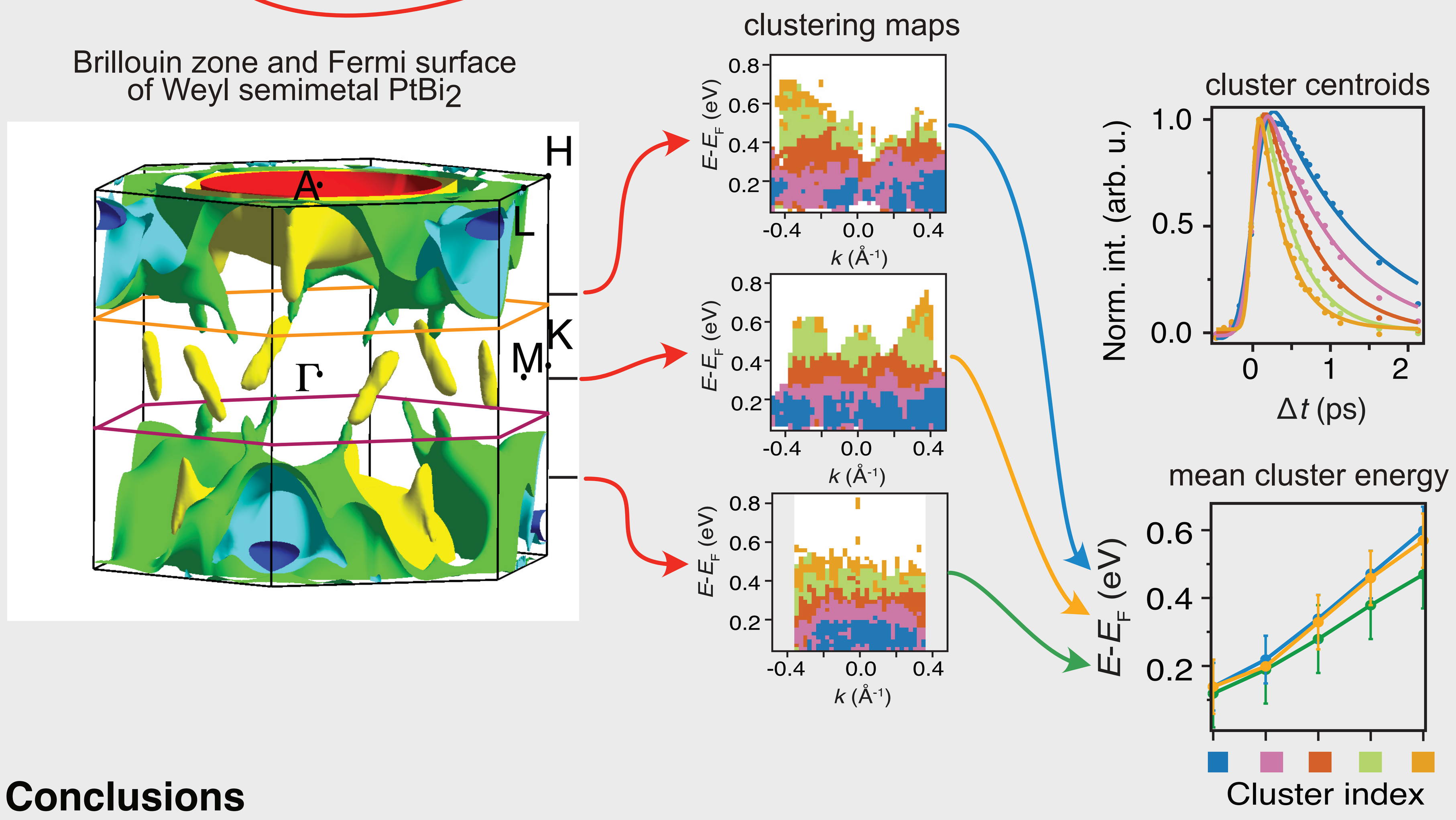
Stein Ymir Agustsson *et al.*, Machine Learning: Science and Technology **6**, 015019 (2025)

Time-resolved ARPES

- Excitation of system with first laser pulse (pump), ARPES with time-delayed second pulse (probe).
- Access to electron dynamics, light-induced ultrafast phase transitions, light-induced transient states of matter.
- More experimental parameters: energy, two emission angles, time delay Δt.
- Objects to be clustered: 1D time distribution curves (TDCs).
- Used here to study difference in electron dynamics throughout 3D Brillouin zone of the Weyl semimetal $PtBi_2$.







Conclusions

- Mean cluster energy lowest for states in the Brillouin zone region with many bulk Fermi surface elements.
  -> Carrier dynamics accelerated by the presence of metallic decay channels.
- High signal / noise cluster centroids.
- No (biased) fitting model required.
- Excellent to find trends in multi-dimensional data.

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