Investigating the insulator to metal transition in $\mathrm{Ca_2RuO_4}$ with k-means

Anders S. Mortensen, Katarina Præst, Davide Curcio, Philip Hofmann

Institute of Physics and Astronomy, Aarhus University

AARHUS UNIVERSITY

Many complex oxides undergo a temperature-driven insulator-to-metal transition (IMT), usually around room temperature. In some materials, an IMT can also be induced by applying a current, opening the possibility to use these materials as controllable switches in electronic devices. $\mathrm{Ca_2RuO_4}$ is such a case: The resistivity can be changed by orders of magnitude when a current is applied, but the underlying physics is poorly understood. In this study, angle-resolved photoemission spectroscopy (ARPES) measurements of the current-induced IMT in $\mathrm{Ca_2RuO_4}$ are clustered with k-means. The qualitative signs of the IMT are correctly identified by the clustering algorithm, both when clustering the full angle and energy-resolved spectra and when clustering the angle-integrated energy distributions. In addition, more detailed information on the changes in the electronic band structure under the IMT is revealed.

The Insulator to Metal Transition in $\mathrm{Ca_2RuO_4}$

- $\mathrm{Ca_2RuO_4}$ can undergo a current or temperature-induced insulator-to-metal transition, with potential applications in electronic devices.
- The exact driving mechanism behind the current-induced IMT is not well understood, but it can be studied with nano-ARPES.

Studying $\mathrm{Ca_2RuO_4}$ with Nano-ARPES

- In nano-ARPES, a nanometre-sized UV light is scanned across the sample. The emission angle and kinetic or binding energy of the resulting photoelectrons are measured. This results in a "map" of the sample, with a spectrum at each pixel.
- A current is passed through the sample to induce the IMT. This also shifts the measured energy.
- The data were measured at the Soleil synchrotron radiation source for ref [1].

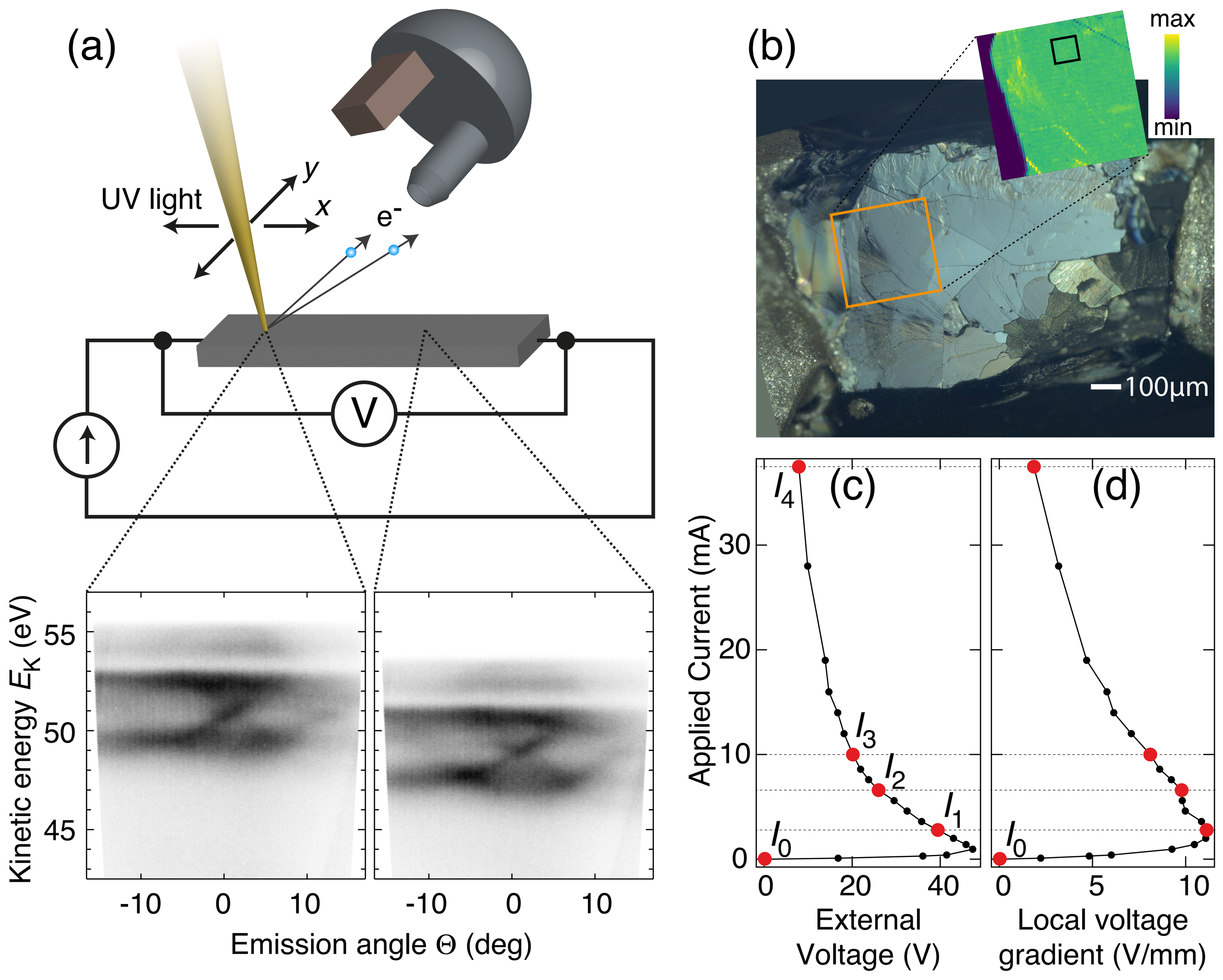

Fig. 1: Figure 1 from ref [1]. a) Sketch of the experimental setup, and two examples of ARPES spectra measured at different positions on the sample. Note the shift in energy. b) Microscopic image of the sample. The orange cutout shows the section of the sample on which the measurements were performed. c) IV-curves measured externally and d) measured locally via the energy displacement of the spectra.

k-means clustering for identifying the IMT

- The metal state has a high density of states (DOS) near E_F compared to the insulating state.
- Summing the signal near E_F in a spectrum can hint at the sample state.
- k-means clustering can identify the IMT if there are overall changes to the DOS, either by clustering the ARPES spectra directly, or just the energy spectrum (EDC).

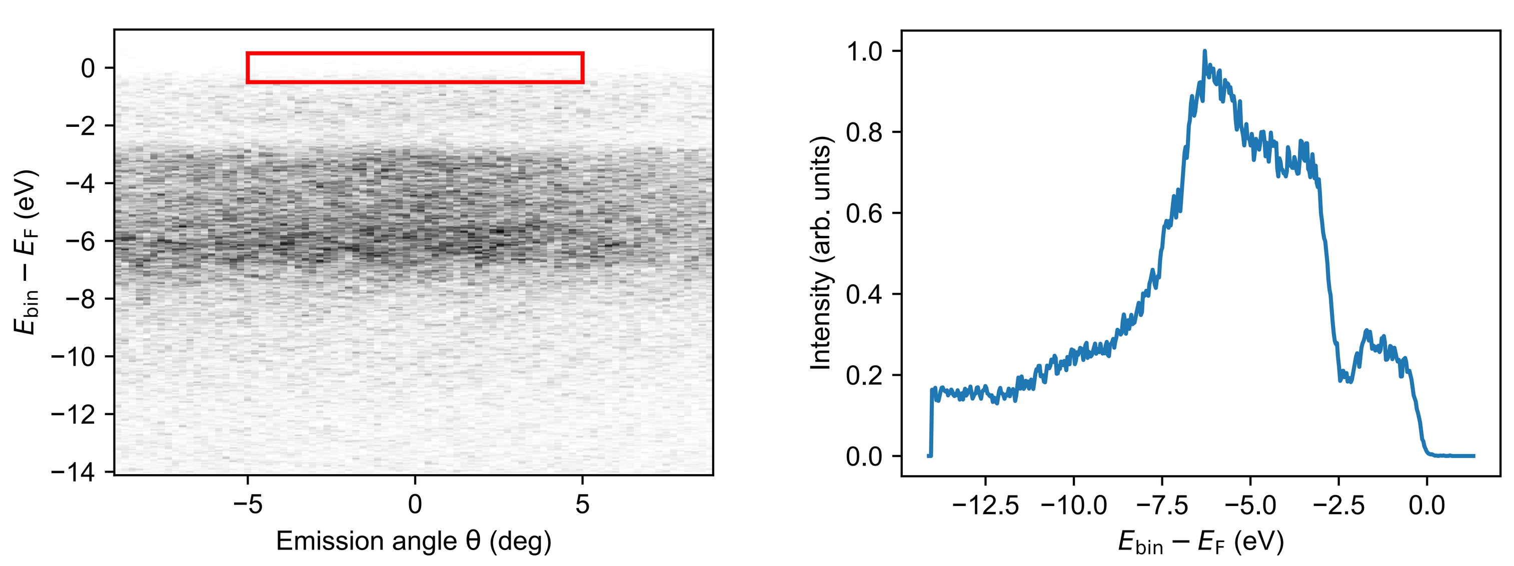

Fig. 2: An example of an ARPES spectrum (left plot), with the area near E_F highlighted, and the corresponding EDC (right plot).

Clustering Results

The clustering was performed on the full ARPES spectra and energy distribution curves(EDCs). **The results are qualitatively similar to those from ref [1].**

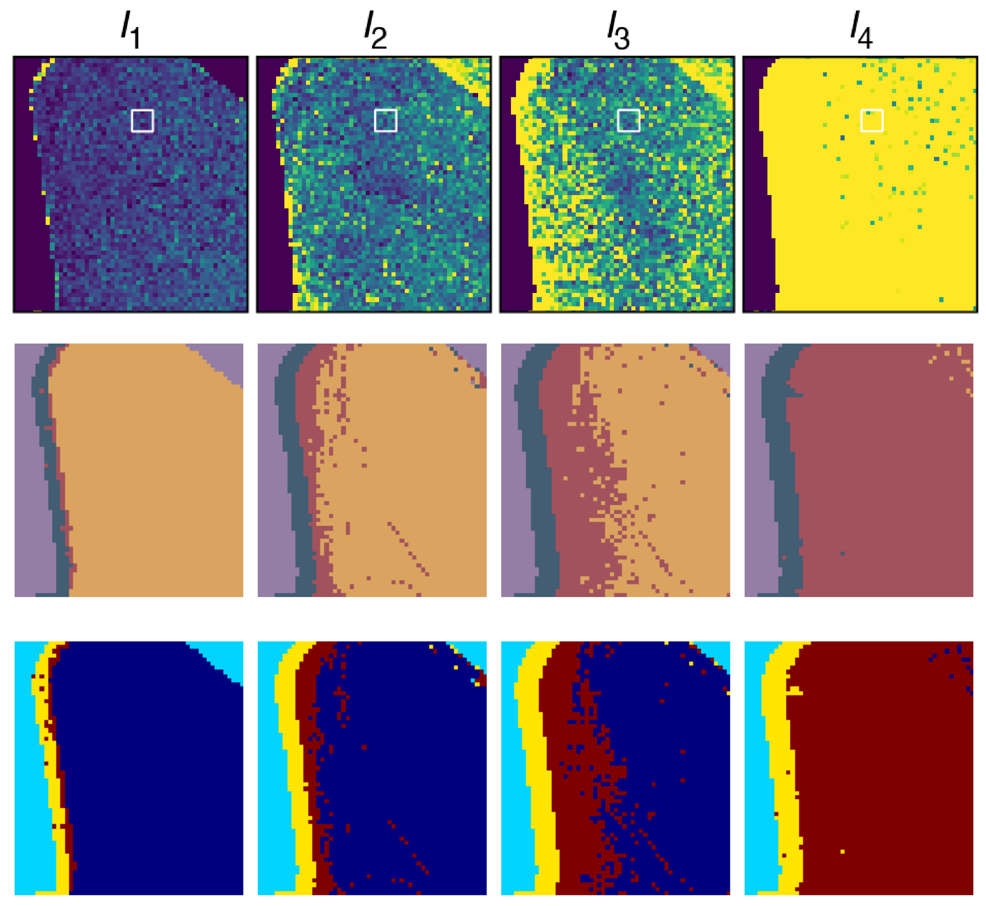

Fig. 3: Top: The main results from ref [1]. The colour corresponds to an integral of the spectra near E_F. Blue is low, yellow is high. Middle: The results from clustering the full spectra. Bottom: The results from clustering the EDCs. In all cases, the result from each spectrum is mapped to the corresponding sample position.

The cluster centroids provide high-statistics measurements of the insulator and metal phases. **The IMT is accompanied by changes in the band structure**, with the most intense bands becoming more diffuse, in addition to the shift at E_F.

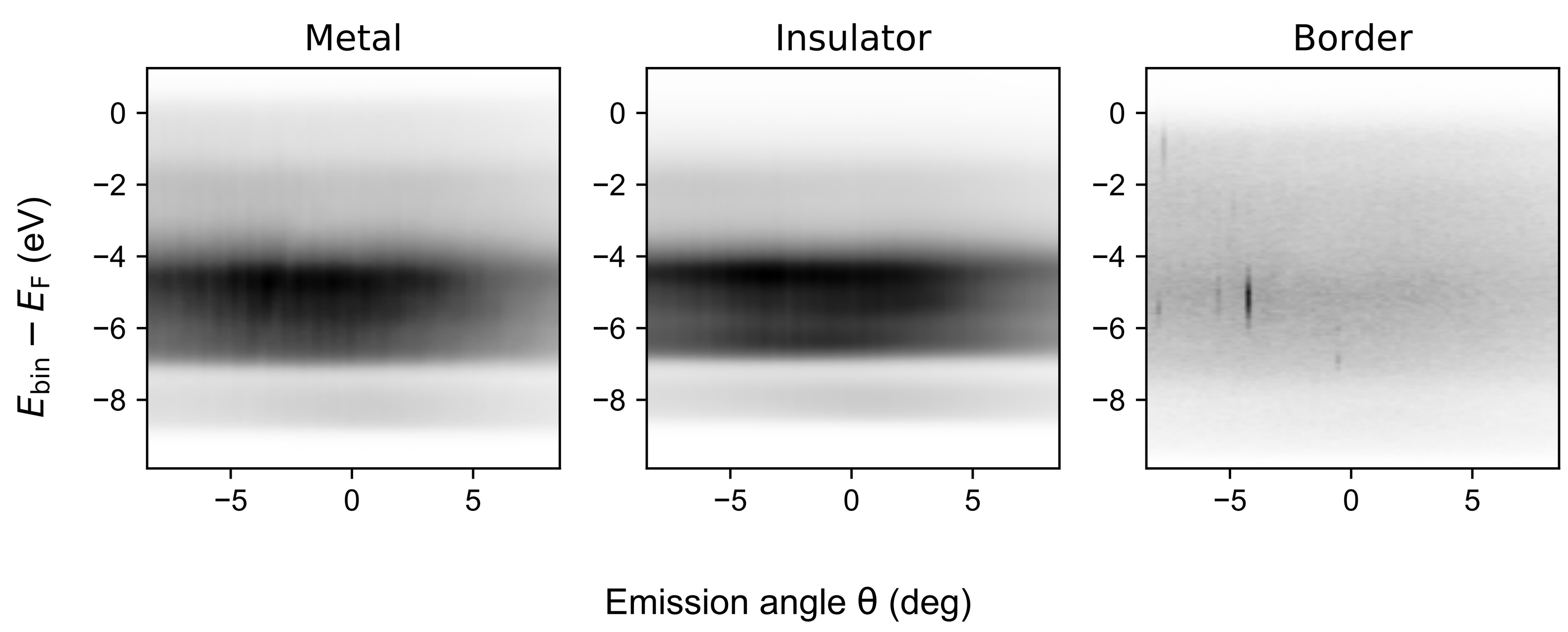

Fig. 4: Cluster centroids from clustering the full spectra.

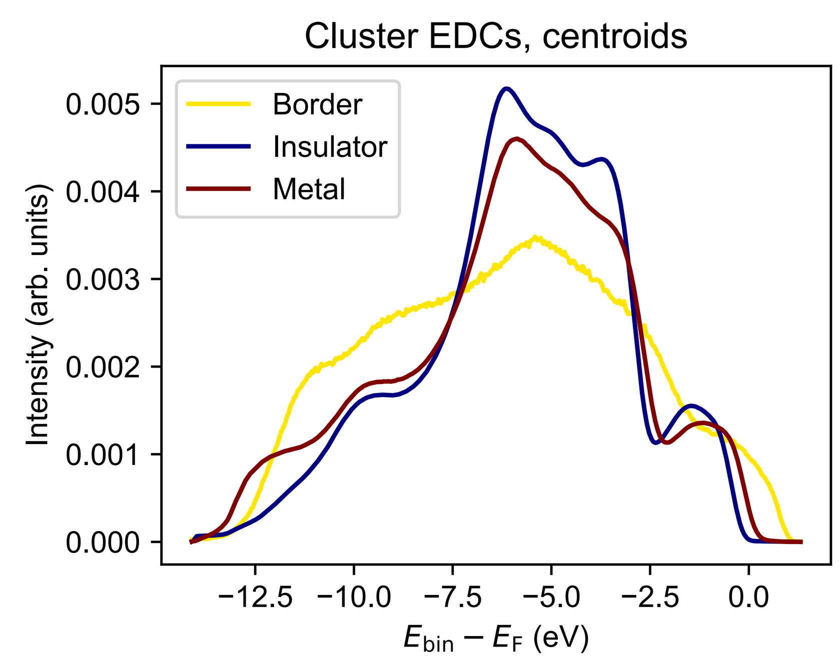

Fig. 5: Cluster centroids from clustering the EDCs

Conclusion and outlook

- The IMT characteristics reported in ref [1] are well reproduced.
- Additional changes in the band structure are observed.
- There is little difference between clustering on the EDCs and the entire spectra.
- The method is novel, and part of an emerging field of applying machine learning to ARPES data, with even simple algorithms proving very powerful.

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References

[1] Davide Curcio et al. "Current-driven insulator-to-metal transition without Mott breakdown in $\mathrm{Ca_2RuO_4}$". In: *Phys. Rev. B* 108 (16 2023), p. L161105.