DFT AND SIMULATION OF THE ARPES EXPERIMENT- AS A WAY TO BETTER UNDERSTAND THE EXPERIMENT

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Theoretical calculations based on the Density Functional Theory (DFT) method are a key technique in materials research, enabling the prediction of electronic structures and properties at the atomic scale. On the other hand, the ARPES (Angle-Resolved Photoemission Spectroscopy) experiment provides direct information about the band structure of electrons in a material. Cooperation between these two approaches can lead to a deeper understanding of electron behavior in the material under investigation.

Our research shows that combining computational data (DFT and ARPES simulations using Chinook software) with analysis of the ARPES experiment leads to better characterization of electron bands in the materials under study. We found that there are cases in which theoretical DFT calculations cannot explain what we observe in the ARPES experiment and therefore we need to simulate it.

Our work underscores the importance of using ARPES simulation (in addition to DFT calculations) when comparing experimental data with the ARPES technique. We show that cooperation between the two approaches can lead to a more complete understanding of the electronic structure of materials, and reveal areas that require further research.

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