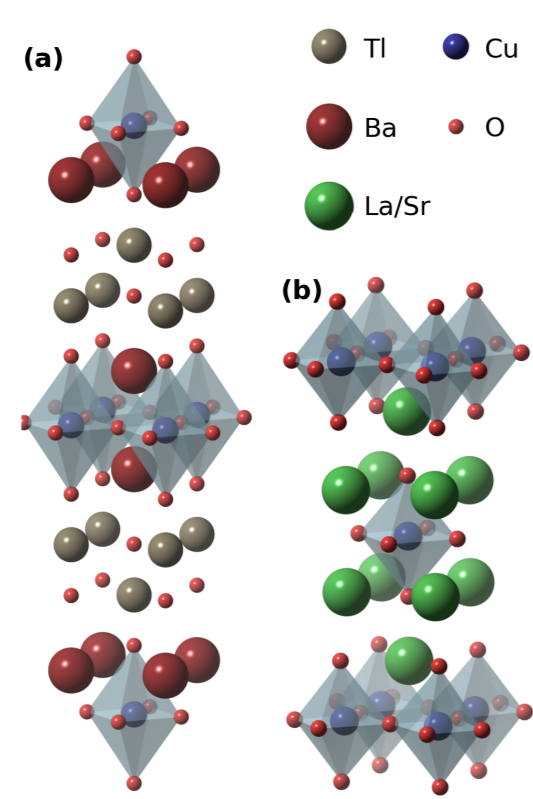


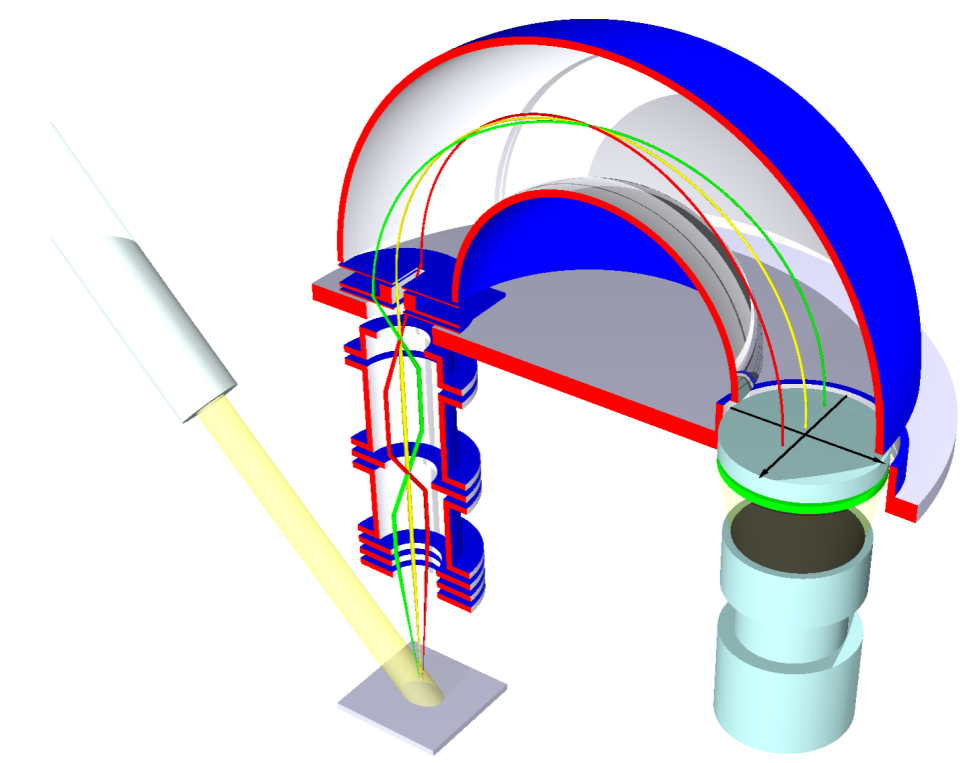
# Comprehensive ARPES and DFT study of overdoped single-layer cuprates



Crystal structures of (a) TI2201 and (b) LSCO.

## Summary

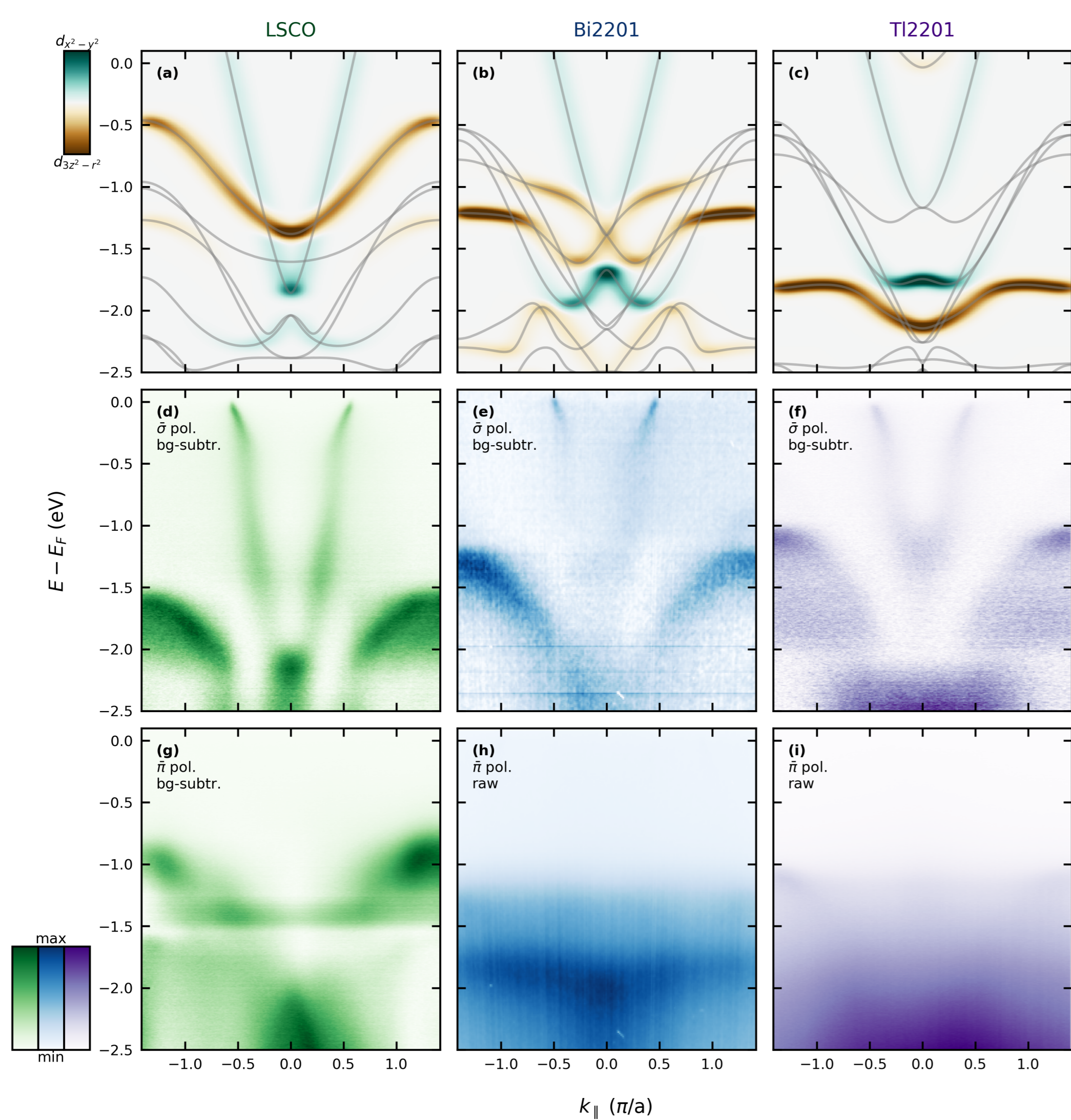
- Examine band structure of four compounds:  $\text{La}_{1.59}\text{Eu}_{0.2}\text{Sr}_{0.21}\text{CuO}_4$  (Eu-LSCO),  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO),  $\text{Bi}_2\text{Sr}_2\text{CuO}_{6+\delta}$  (Bi2201) and  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$  (TI2201) with ARPES and DFT.
- Compare trends of band positions with apical oxygen distance  $d_A$  between experimentally obtained and calculated data.
- DFT captures many aspects of the measured band structure, but overestimates band positions, especially of the  $d_{3z^2-r^2}$  band.



Scheme of the ARPES experiment.

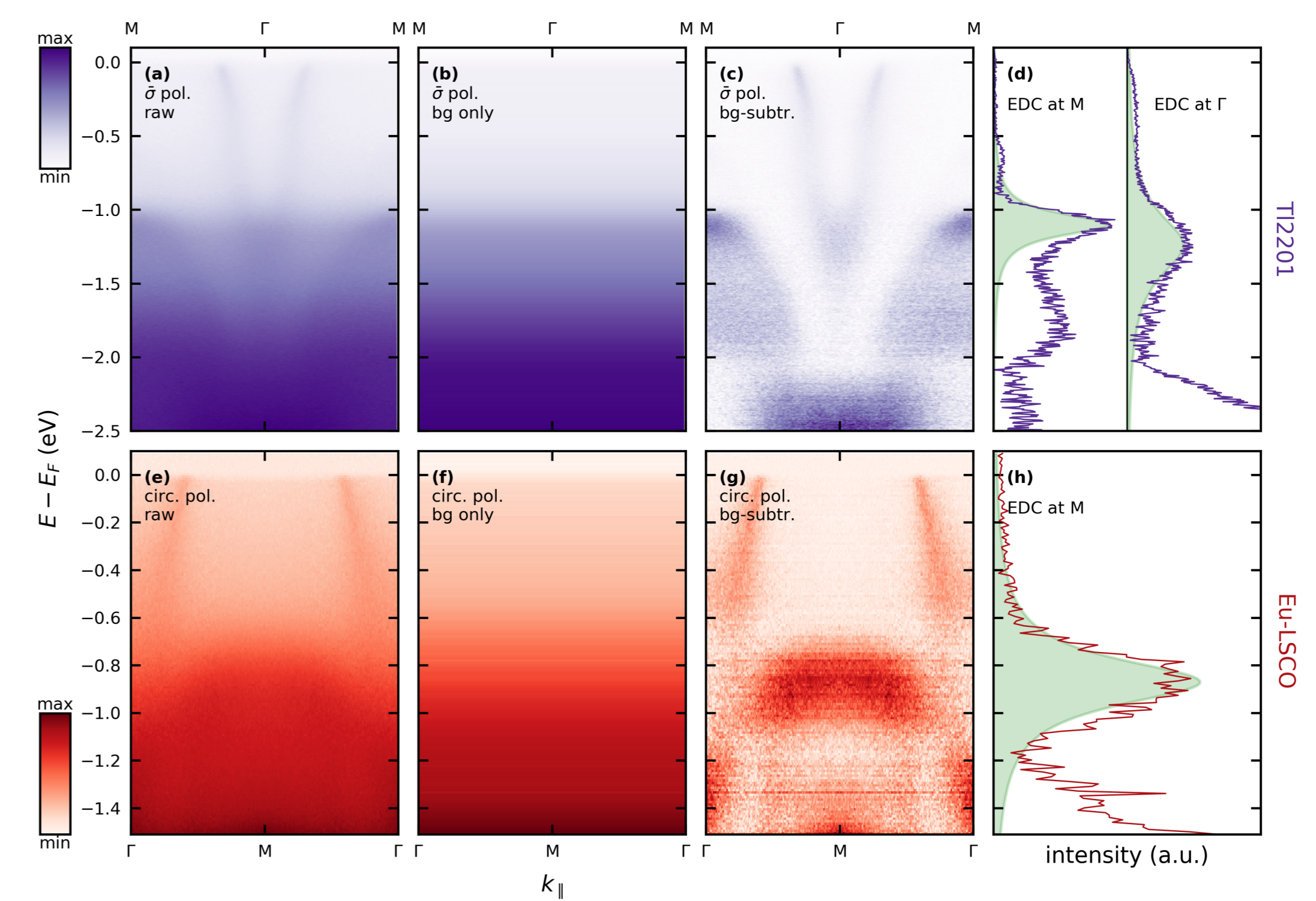
## Experimental and calculated data

Bands with odd (even) symmetry with respect to the photoemission mirror plane are suppressed when exciting with perpendicularly (parallel) polarized X-rays. This allows identification of bands with specific orbital character.



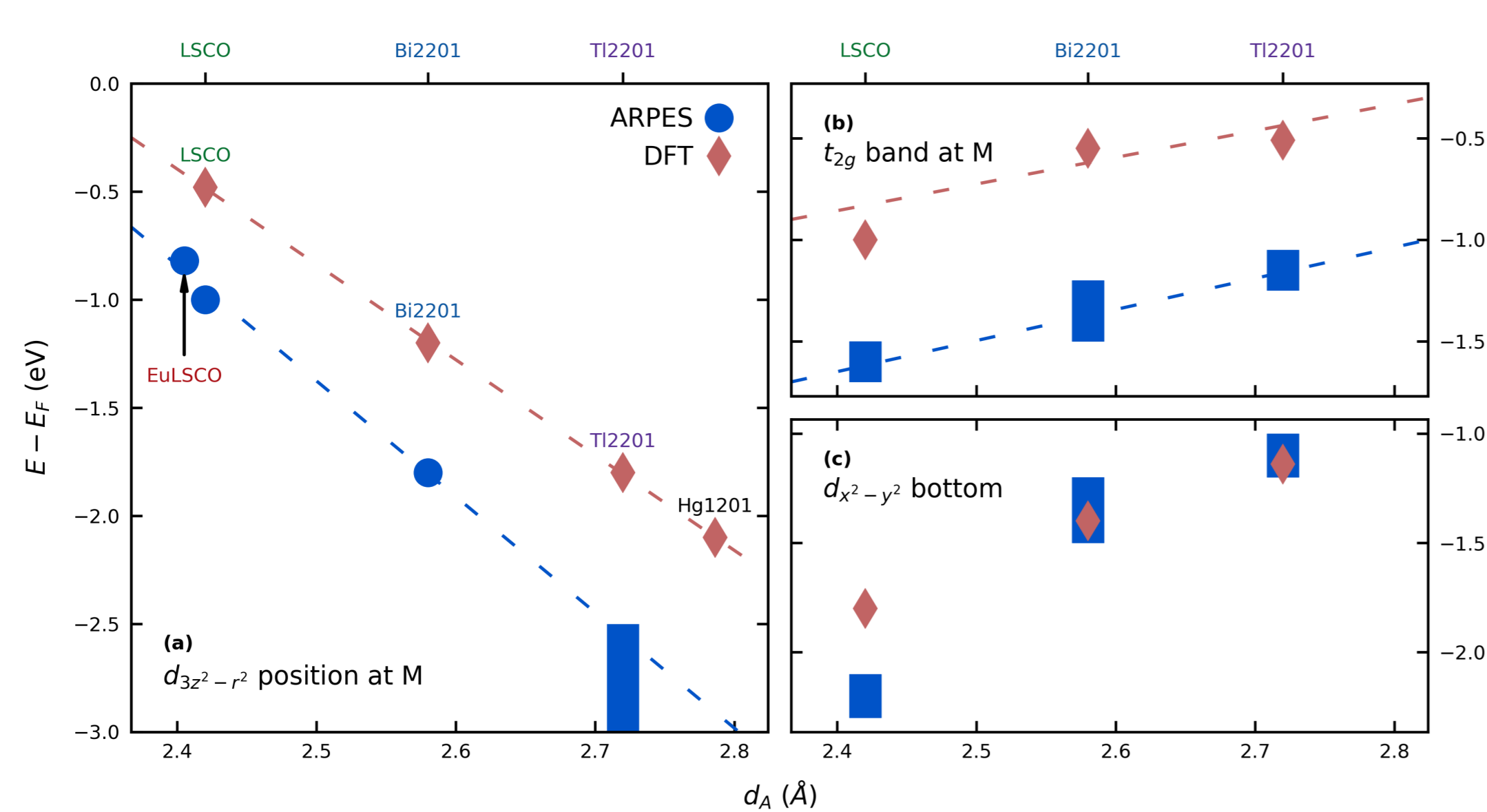
## Background subtraction

A background profile is created by taking the mean of the 5 lowest values in each MDC. Subtracting the thus generated profile enhances the visibility of dispersive bands. There is a caveat, however: flat bands get canceled out with this methodology.



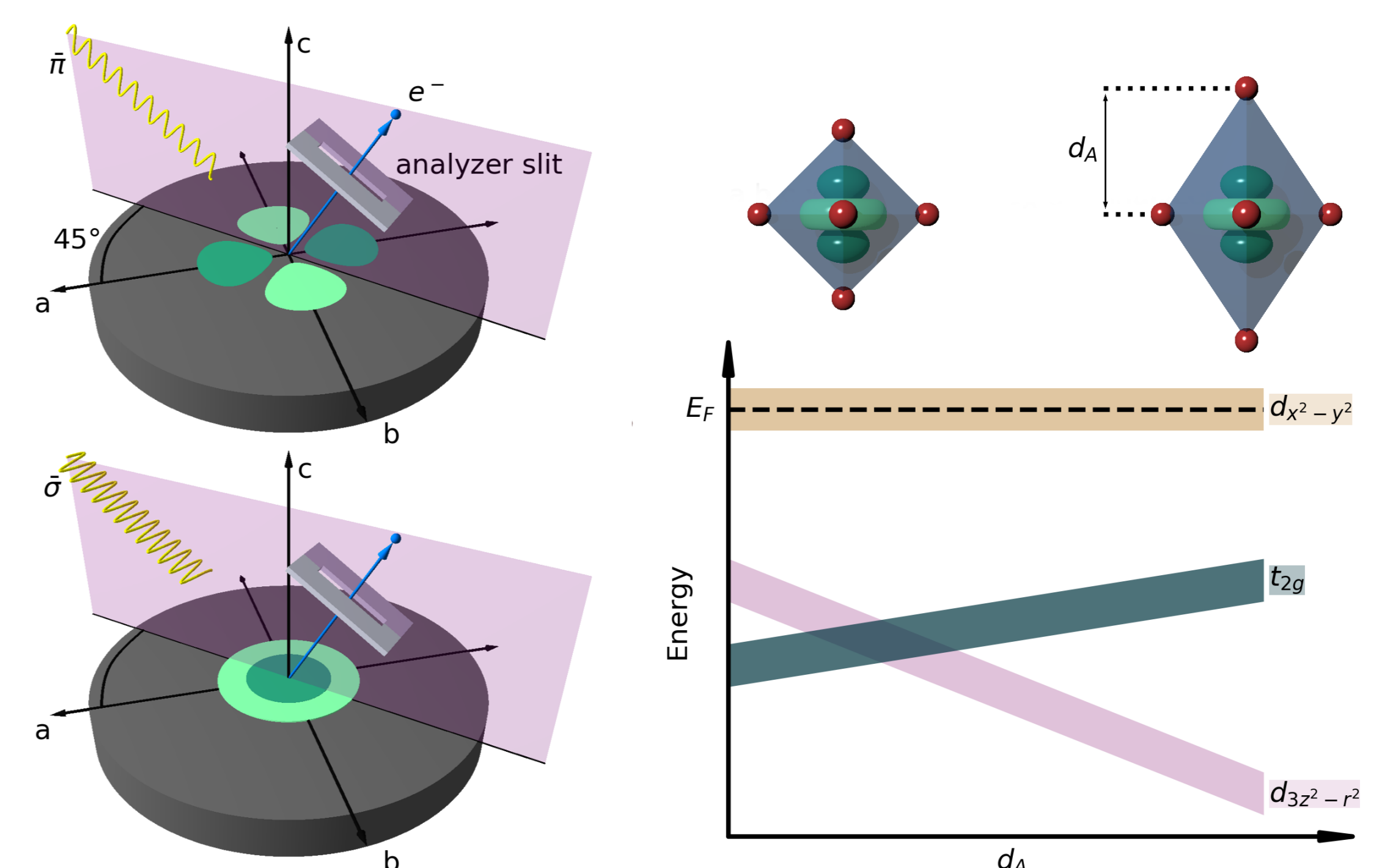
## DFT versus Experiment

Surprisingly, DFT captures many trends of the bandstructure qualitatively. The quantitative discrepancies provide a target for an improvement of the DFT methodology applied to the cuprates.



## Incident polarization and the apical oxygen distance $d_A$

Presented below are schematics of the photoemission mirror plane in the nodal orientation (left). Two case for  $\bar{\sigma}$  and  $\bar{\pi}$  polarized light are indicated and the projections of the  $d_{x^2-y^2}$  and the  $d_{3z^2-r^2}$  orbitals are depicted as well. Right: The effect of tetragonal distortion (increase of  $d_A$ ) on the energy of the  $d_{3z^2-r^2}$  orbital.



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