Photoemission final states in a one-step-model applied to molecular thin films

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We present a method for the calculation of photoemission matrix elements for molecular thin films which goes beyond the currently prevalent plane-wave-approximation. It is illustrated on the example of pentacene mono- and bilayers on a silver crystal where we can track the layer-by-layer structural evolution within the thin film away from the interface. The procedure utilizes **A**ngle-**R**esolved **P**hoto**E**mission **S**pectroscopy (ARPES) [1] combined with simulations within an **I**ndependent **A**tomic **C**entre (IAC) framework [2]. It is based on and expands previous work which looked into the structural evaluation of systems with a single kind of molecular geometry [3],[4],[5].

Both measurement and simulation are quick and straight-forward to perform and evaluate. The approach provides high accuracy, is suitable for a wide range of systems and can be extended to include further effects in a modular manner.

Time permitting, we will briefly look into the application of this model to more complicated systems, specifically non-planar molecules and those involving substantial electron scattering.

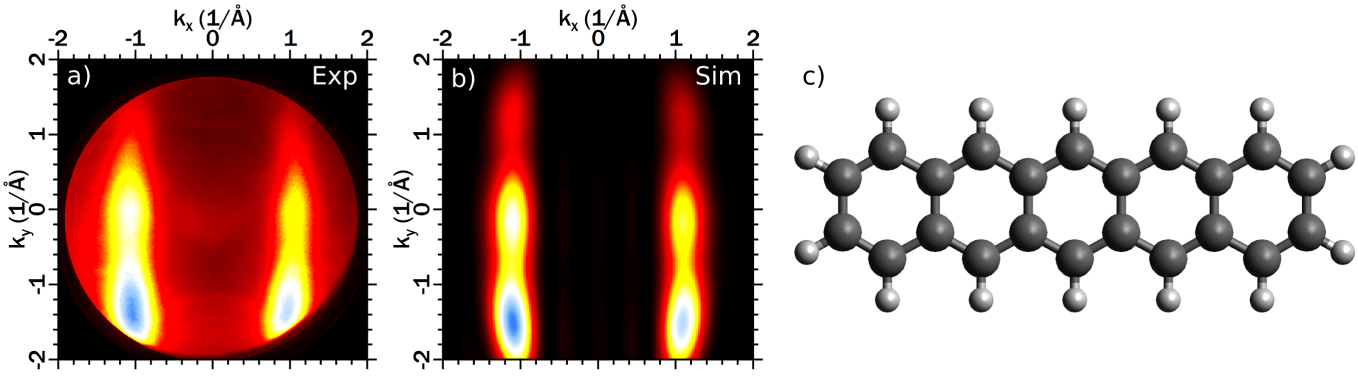

FIG. 1. a) Experimental angle-resolved photoemission intensity in reciprocal space of a pentacene bilayer illuminated by p-polarized light at $E_{ph} = 40\ eV$. The light incidence is from above, in the direction of negative y-values and slightly negative x-values. b) Ab-initio simulated photoemission intensity in reciprocal space under the same conditions used in the experiment. c) Isolated pentacene molecule in realspace where black spheres equal carbon atoms, grey ones equal hydrogen atoms.

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