

FIG. 3: (a) Result of a tight-binding calculation for a σ -type band formed from the C 1s core states in graphene. The bonding (blue) and anti-bonding (red) bands are degenerate at \bar{K} and show the highest splitting at $\bar{\Gamma}$. The inset shows the Brillouin zone of graphene. (b) and (c) Calculated photoemission intensity from all the anti-bonding and bonding states, respectively. The grey-scale is chosen such that bright corresponds to high intensity. The green crosses mark the reciprocal lattice of graphene and the green hexagon the first Brillouin zone. (d)-(f) Calculated photoemission intensity from the states in the binding energy windows indicated by the small circles in (a). Note the similarity of the emission pattern from the bonding states in (d) with the positions of maximum binding energy in the right panel of Fig. 2.

the non-linear dispersion away from \bar{K} . The photoemission intensity around this triangular contour shows strong variations which are caused by the interference effect and very similar to the results obtained for the valence π -band of graphite and graphene [4, 5].

As already expected from Fig. 3(b) and (c), the interference effect is even stronger for emission from the bonding and anti-bonding states at $\bar{\Gamma}$ (see Fig. 3(d) and (e)). The intensity variations of both bands are almost opposite to each other: for some $\bar{\Gamma}$ points only the bonding band is observed, for others only the anti-bonding band. For normal emission this is easy to understand: for the bonding band the wave functions centred on the two atoms in the unit cell emit in phase and this band is observed. For the anti-bonding wave function, the two atomic wave functions emit out of phase, thus suppressing the photoemission.