The Electronic structure of 2D materials

Look to Symmetry and Thermodynamics: Chemistry is everything !

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The MoS_2 and WSe_2 monolayers are a direct gap semiconductor and promising for possible 2-dimensional spintronic devices and graphene heavily investigated for such devices. But symmetry, as well as the nature of the band gap (direct or indirect) matters. While there are both experimental and theoretical studies of the band structure of $MoS_2(0001)$ and $WSe_2(0001)$, as well as for monolayer MoS_2, few (actually none in any significant fashion) have considered the wave vector dependent symmetry and origin of the spectral weights. We have undertaken angle-resolved inverse photoemission and photoemission spectroscopy measurements to identify the wave vector dependent band structure of $MoS_2(0001)$ [1], $WSe_2(0001)$, graphene and the influence of various contact materials using p- and s-polarization geometry to distinguish the even and odd states. Indeed, these are the first combined angle-resolved photoemission (occupied state) and angle-resolved inverse photoemission (unoccupied state) studies of the transition metal dichalcogenide reported. Fig. 1 shows the wave vector and symmetry dependent band structure of $MoS_2(0001)$. Through comparison with the density functional theory (DFT) calculations, the experimental results for p- and s-polarization geometries, can be assigned to a particular symmetry with good agreement. The dispersion of several bands are easily discerned and we find that the symmetry is in fact wave vector dependent due to overlapping wave vector dependent spectral weight contributions.

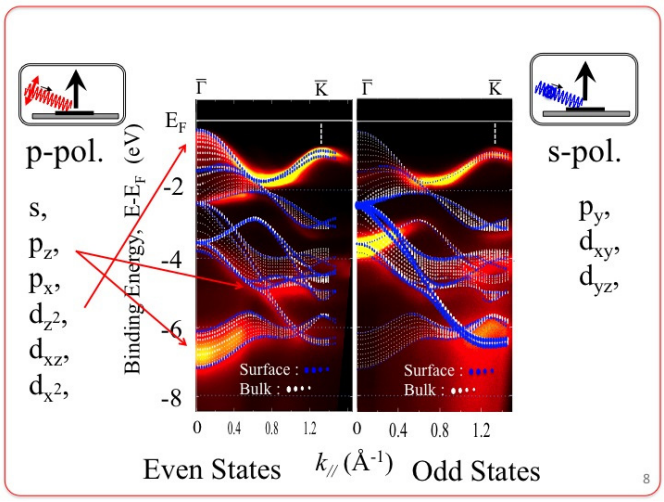

Figure 1. Comparison of both the nominally even (left) and odd (right) symmetry band structure obtained from density function theory (DFT) and experiment. Adapted from [1].

Na atoms donate electrons to MoS_2 [2] or WSe_2. Surprisingly, Na adsorption does not significantly perturb the MoS_2 or WSe_2 band dispersion, and the band shifts are close to rigid. Cobalt is far more strongly interacting with WSe_2, but even with very low coverages is seen to be a p-type dopant. Even gold, a standard contact material will dope many 2D materials.

References:

[1] T. Komesu, et al., *J. Phys.: Condens. Matter* **26** (2014) 455501.
[2] T. Komesu, et al., *Applied Physics Letters* **105** (2014) 241602.