Graphene functionalization with nitrogen and oxygen: controlled modification of the electronic properties

1 PETER BROMMER, ALEXANDER MARSDEN, NEIL WILSON, GAVIN BELL, DAVID QUIGLEY, Department of Physics, University of Warwick — For many applications it is essential to modify the electronic properties of graphene in a controlled fashion. This can be achieved via oxygen and nitrogen functionalization in ultra-high vacuum, leading to a system in which electronic and structural properties can be systematically studied. Here we present insights from DFT calculations on functionalized graphene systems, such as the low-energy configurations and simulated transmission electron microscopy (TEM) images, binding energies and effective band structures (EBS) of the N and O decorated graphene sheets. We directly compare our results with experiments on CVD grown graphene. Angle-resolved photoemission spectroscopy (ARPES - performed at the Antares beamline of Synchrotron SOLEIL, France) resolves the band structure changes on functionalization, whilst the simulated TEM images provide feedback for the interpretation of low-voltage aberration-corrected TEM measurements. Combined, the computational and experimental results have important implications for the manipulation of electronic properties in graphene by controlled functionalization.

1We acknowledge funding by the EPSRC through grant number EP/H00341X/1.