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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.

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