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A theoretical study of chemical functionalisation of graphene: graphane and graphXene

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Chemical functionalisation of graphene is reported from a first principles, theoretical study [1]. The electronic structure, including band gap, of H adsorbed on graphene (i.e. graphane) is discussed in this presentation [2]. In addition, adsorption of Group VII elements on graphane (named graphXene) is also reported [3]. Similarities and differences in the chemical binding and electronic structure of graphane and graphXene are analyzed. The adsorption on graphene is found to, depending on adatoms, result in sp2 or sp3 binding, where in general the sp3 bonded systems show a bandgap. The theoretical calculations make use of both GGA functionals as well as the GW approximation. In addition to large graphene layers, theoretical analysis of functionalised graphene nano-ribbons will also be presented [4]. References:

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[4] S. Bhandary, et al., Phys. Rev. B 82, 165405 (2010).