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Band Engineering of Graphene using Metal Mediated Oxidation

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In the study of materials for electronic devices, there is a continuous search for new materials with useful properties such as grapheme and grapheme-based materials. Research on these materials is widespread for many applications such as manipulation the band structure of grapheme to induce a semiconducting band gap. The focus of this study is a cobalt nanoparticle-graphene system investigated for the manipulation of the graphene electronic structure. The properties of this system were investigated using various X-ray spectroscopy and surface science techniques. At a low concentration of cobalt, the metal is completely oxidized into primarily CoO, and the graphene is not heavily damaged. Oxide groups form on the graphene surface but are found to be proportional to the cobalt concentration at thicknesses below 1 nm. Using X-ray spectroscopy, an electronic band gap of up to 0.30 eV is observed in graphene 2p states when cobalt nucleates into nanoparticle islands on the graphene surface. The mechanism of band gap opening is interpreted using electronic structure calculations, showing a contribution from both the oxidation of the graphene itself and the presence of CoO that acts to localize electron charge. These results have implications for graphene electronics and spintronics where magnetic metals can be used to induce a band gap in graphene that is stable at room temperature and under atmospheric exposure.

[1] Paul F. Bazylewski, Van Luan Nguyen, Robert P.C. Bauer, Adrian H. Hunt, Eamon J. G. McDermott, Brett D. Leedahl, Andrey I. Kukhareno, Seif O. Cholakh, Ernst Z. Kurmaev, Peter Blaha, Alexander Moewes, Young Hee Lee, and Gap Soo Chang. *Sci Rep.* 2015, 5, 15380.

[2] P. Bazylewski, D. W. Boukhalov, A. I. Kukhareno, E. Z. Kurmaev, A. Hunt, A. Moewes, Y. H. Lee, S. O. Cholakh and G. S. Chang. *RSC Adv.*, 2015, 5, 75600-75606.

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