
**BUCKLING, FOLDING AND RIPPLING OF
GRAPHENE NANORIBBON EDGES****C. P. Ewels^{a*}, Ph. Wagner^a, V. Ivanovskaya^a and P. R. Briddon^b**^aInstitut des Matériaux Jean Rouxel (IMN), Université de Nantes,
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Creating an interface in a material often leads to bond reconstruction and functionalisation, resulting in different interface properties such as lattice parameter to that of the bulk. In conventional 3D semiconductor materials any resultant lattice mismatch strain can be compensated through the production of dislocations. However two dimensional layered materials such as graphene have an alternative mechanism for relieving edge-induced strain, namely, structural deformation into the third dimension via rippling or buckling [1].

This additional degree of freedom adds significant richness to graphene edge chemistry, which we investigate here for armchair graphene nanoribbons (a-GNRs) using the example of hydroxyl functionalisation. Local rippling induces strong effects on the structural, electronic, chemical and mechanical properties of the nanoribbon. The study points the way towards "edge termination engineering" as a way to create graphene nanoribbons (GNRs) with custom designed properties [2].

Aberration corrected high resolution electron microscopy studies have pushed the study of non-functionalised graphene edges [3], and a variety of alternative edge structures have been both observed and theoretically proposed [4]. We discuss the possibilities proposed in the literature and their effect on the electronic and structural ribbon behaviour, and extend the range to include several new edge structures not previously considered. In particular we identify a new thermodynamic ground state for unterminated edges where the sheets are folded back and bond into themselves, producing 'nanotube'-like edge terminations separated from the bulk graphene layer via a line of sp³-coordinated carbon atoms [5]. [6-7]

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- [7] A full publication list including downloads is available at www.ewels.info