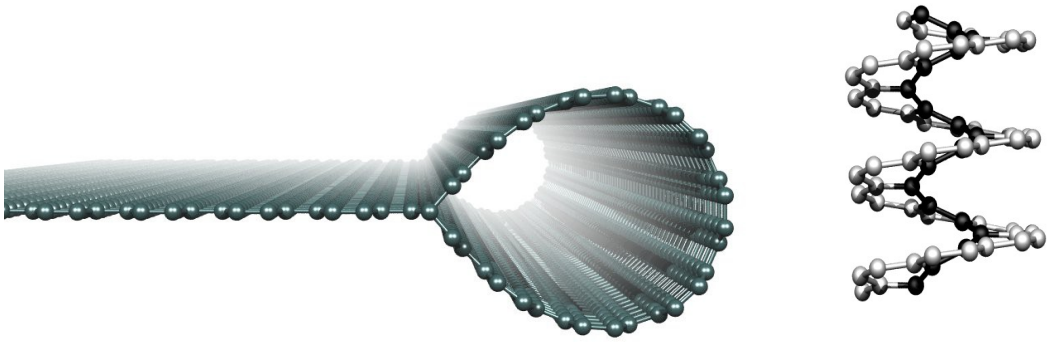
Tuning Carbon Nanomaterial interfaces : DFT simulation and experiment

Chris Ewels

IMN, CNRS UMR6502, 2 Rue de la Houssiniere, BP 32229, 44322 Nantes, France

chris.ewels@cnrs-imn.fr



Interface formation in three-dimensional crystal lattices involves well characterised processes such as rebonding and rehybridisation, localised strain and dislocation formation. In contrast two dimensional crystal lattices, of which graphene is the archetype, are terminated by lines, and the additional available dimension opens up new topological interfacial possibilities.

We show via DFT and DFTB [1] calculations that graphene sheet edges can adopt a range of topological distortions depending on their nature. Rehybridisation, local bond reordering, chemical functionalisation with bulky, charged, or multi-functional groups can lead to edge buckling to relieve strain [2], folding, rolling [3] and even tube formation [4]. We show how careful edge design during synthesis and post-processing can lead to a new class of highly tuneable and robust graphene ribbon types.

I discuss future areas where we expect collaboration between DFT simulation and experimental characterisation to open exciting new opportunities in carbon nanomaterial research [2,3].

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References

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