**Computational studies of graphene and nitrogen-doped graphene as functional two-dimensional materials**

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Graphite, graphene and their doped variants have important applications including materials for battery electrodes, microelectronic components and catalysis. These properties will be very sensitive to the structure of the material as well as the doping content and the type of doping. Therefore it is of great significance to develop approaches for fabrication of these materials with well-controlled specifications. For example, nitrogen doping of graphene can be used to tune the properties of the material including their electronic properties and their interactions with adsorbates.

We will discuss how computations can be used to help select experimental conditions so that the desire structures are attained in fabrication. We will consider cases where the catalyst used for growth of the material is tuned and other cases where the feedstock can be tuned. This will include the size of the two-dimensional single-crystal materials, and the type of doping. For example, the growth of large area single‐crystalline graphene is catalysed by CuNi alloys and the size and the nucleation density of the graphene can be changed by changing the Ni content of the alloy. These results can be fully explained using computational methods.1

We will also discuss how the properties of the materials can be tuned by doping and stacking of the two-dimensional materials.

**References**

1. Liu Y, Wu T, Yin Y, Zhang X, Yu Q, Searles DJ, Ding F, & Yuan, Q (2018). How low nucleation density of graphene on CuNi alloy is achieved. Advanced Science 5 (6), 1700961.