First-principles electronic and structural properties of BNC nanomaterials

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Advanced Silicon-based device components are moderately chemically tunable, which restricts the realistic prospect of current technology transitioning into flexible and miniaturized devices. Graphene is a promising candidate [1] to replace Silicon as semiconducting material and heteroatom co-doping has emerged as an appealing strategy to tune its electronic and structural properties. Since the existing BN-doped carbon-based materials are not periodically doped, their properties are not reproducible [2] hence a substantial challenge is to gain control in the incorporation of these BN rings in a reproducible manner. The present study aims to search for an entirely new class of BCN hybrid 2D materials in order to construct a high-accuracy reference database with key electronic and optical properties. This goal is achieved by using *ab initio* quantum mechanical calculations relying on density functional theory (DFT) and many-body perturbation theory (MBPT). A large set of BNC materials exhibiting different doping parameters (Figure 1) is considered in order to search for the best configuration in terms of both stability and band gap. These models are then compared to benchmark systems, displaying high stability. The corresponding cohesive energy presents comparable values and well-defined linear trends with BN-ring concentration. Within the same doping patterns, different ring orientations are also considered suggesting that the cohesive energy does not qualitatively change. On the other hand, the band gap is found to be sensitive on the doping pattern and its value is considerably higher when BN rings are in the same orientation.

References

[1] K. Novoselov, *et al.,* Nature **490**, 192-200 (2012).
[2] L. Ci, *et al.*, Nat. Mater. **9**, 430-435 (2010).

Figures

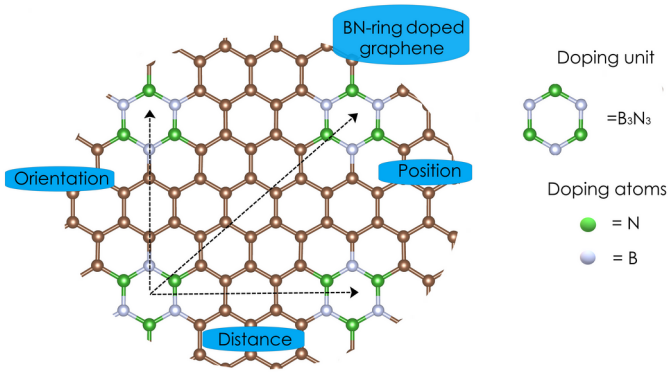

Figure 1: BN-ring doped Graphene. Different doping parameters, such as orientation, position and distance, are considered herewith to search for an optimal doping configuration in terms of stability and band gap in order to possibly replace Silicon in future opto-electronic nanodevices.