First-principles study of the structural and electronic properties of BN-ring doped graphene

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Since advanced silicon-based device components are moderately chemically tunable, doped graphene has emerged as a promising candidate [1] to replace this semiconducting material in flexible miniaturized electronic devices. Indeed, heteroatom codoping (i.e., with boron and/or nitrogen) is an appealing strategy to tune both its structural and electronic properties, possibly inducing a band gap in graphene. However, presently synthesized BN-doped carbon-based materials are randomly doped, leading their electronic properties not to be reproducible [2]. Using first-principles techniques, the present study investigates the periodic doping of graphene with borazine-like rings in order to search for an entirely new class of BNC hybrid 2D materials exhibiting high stabilities and optimized band gaps for optoelectronic applications. *Ab initio* calculations show that BN-ring doped graphene displays cohesive energies comparable with benchmark ideal periodic BNC systems (such as BC_3 and BC_2N) with a decreasing linear trend toward high concentrations of BN rings. Band gaps of BN-ring doped graphene systems are calculated using many-body perturbation techniques and are found to be sensitive to the doping pattern and to be considerably larger for high concentration of BN rings exhibiting the same orientation. These predictions suggest that BN-ring doped graphene materials could be interesting candidates for the next generation of optoelectronic devices and open new opportunities for their synthesis using chemical bottom-up approaches.

References

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

Figures

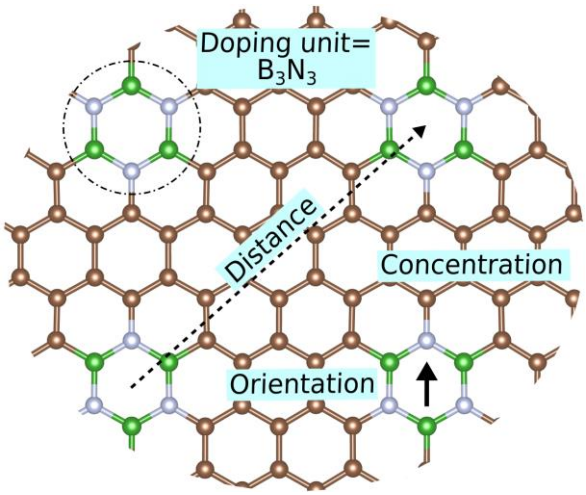

Figure 1: BN-ring doped Graphene. Different doping parameters, such as orientation, concentration and distance, are considered herewith to search for an optimal doping configuration in terms of stability and band gap in order to possibly replace Silicon in future opto-electronic nanodevices.