

# Irradiation effects in carbon and boron-nitride nanostructures: an insight from atomistic simulations

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## ABSTRACT

The irradiation of solids with energetic particles such as electrons or ions is associated with disorder, normally an undesirable phenomenon. However, recent experiments [1] on the bombardment of various nanostructures with energetic particles demonstrate that irradiation can have beneficial effects and that electron or ion beams may serve as tools to change the morphology and tailor mechanical, electronic and even magnetic properties of nanostructured systems.

We systematically study irradiation effects in graphene and carbon nanotubes. By employing various atomistic models ranging from empirical potentials to time-dependent density functional theory, we simulate collisions of energetic particles with carbon nanostructures, and calculate the properties of the irradiated systems. In this presentation, our latest theoretical (and some experimental) results on the response of carbon nanotubes and graphene to electron and ion irradiation will be presented. We will also address the interaction of transition metal atoms with pristine and defected graphene sheets and nanotubes and identify possible avenues for tailoring the electronic and magnetic structure of graphene by irradiation-induced defects and metal atoms. Finally we touch upon the response of BN nanotubes and sheets to ion and electron irradiation.

## References

[1] Krasheninnikov, A. V. and F. Banhart. Engineering of nanostructured carbon materials with electron or ion beams. *Nature Materials*, 6, 2007