MA14-009 - Variational Modeling of Carbon Nanostructures

Abstract

Carbon nanostructures such as graphene, nanotubes, and fullerenes show extraordinary electromechanical properties which make them extremely promising materials in a wide variety of applications from chemistry to nanoelectronics, optics and mechanics. Despite their groundbreaking relevance, a number of fundamental issues concerning geometry, mechanics, and defects in these nanostructures are still largely unexplored from the mathematical point of view. Within this project, we make a multidisciplinary effort towards a comprehensive understanding of these structures, both in their ideal crystalline form and in the presence of defects. To achieve this, we combine variational modelling with state-of-the-art electron microscopy and computational physics. Grounded on variational methods for atomistic models, our methodology will reside on the minimization of suitable configurational potentials including two- and three-body interaction terms. We aim at describing the fine geometry of carbon nanostructures by focusing on local strict minimizers of configurational potentials. This will in particular lead to novel geometric models for carbon nanotubes and fullerenes. We will assess the validity of the Cauchy-Born hypothesis and discuss the mechanical response. Finally, we shall theoretically and experimentally investigate the onset and stability of defects in graphene. Due to the foreseen significance of the studied materials in several fields of applications in the nearest future, our results can be expected to have a relevant impact on next-generation real-life technologies such as touch screens, batteries, fuel and solar cells, and sensors.

Scientific disciplines:
Mathematical physics (60%) | Nanomaterials (40%)

Keywords:
Variational methods, Carbon Nanostructures, Geometry and Mechanics, Stability, Defects

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Further links to the persons involved and to the project can be found under
https://www.wwtf.at/funding/programmes/past/ma/MA14-009/