Project overview:
Nanomechanics for graphene membranes

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(Dated: 28/9-2017)

Background Since the isolation and characterisation of Graphene in 2004 by Andre Geim and Konstantin Novoselov, scientists have marvelled over the physical properties and potential application of Graphene. Being a relatively new material, many aspects and ideas are being investigated and researched at all times. Graphene yield extreme tensile strength as well as extreme electric conductivity, yet its structure is fairly simple. Graphene consists solely of carbon atoms thus making it, as carbon atoms are greatly understood in terms of chemical bonding, easy to simulate using specialised software. As graphene is a very versatile material the possibilities for research in simulation enviroments are virtually limitless. Therefore it is basically possible to make experiments limited only by imagination, in order to discover new properties and possible applications of graphene. This saves ressources before entering the lab, where where the simulated reality is tested.

Purpose A graphene layer on top of a substrate with different sized and shaped holes, would form a nanomembrane. It is expected possible to create such a nanomembrane at the size of few tens of nanometers at Nanotech with Block-copolymer lithography or TEM structuring of a substrate. In a virtual enviroment, it is possible to simulate phonons in the graphene atop of these holes in the membrane. The purpose of this project is to simulate phonons in the nanomembrane and find the optimal conditions for producing phonons in the terahertz spectrum.

Method We will employ the software Atomistic ToolKit (ATK) to calculate phonon properties of membranes as well as performing molecular dynamics of the excited membrane. The software will enable prompt setup of relevant structures so that more time is free to analysis and actual simulations.

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