

Summer Research Program 2011/2012

Project Title *Computational modelling of graphene and related materials*

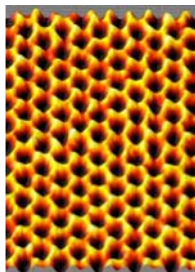
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Objective *Computational modelling of graphene and related materials*

Do you want to learn and discover *something new* about nanoscale materials using advanced computational methods?

Then perhaps you would like to work in the **Laboratory of Computational Mechanics and Materials Science** for your summer research projects!

(a)



(b)

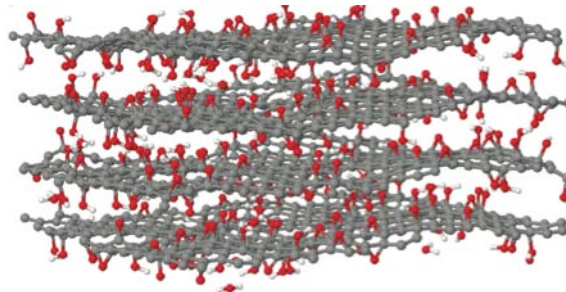


Figure. (a) A Scanning Tunneling Microscopy image illustrating graphene hexagonal lattice, (b) Atomistic model of graphene oxide composite.

Computational Modelling is an analysis technique used to simulate—on computers—any physical system as close to reality as possible in order to understand its behavior and the underlying factors that control it. We have two summer research projects on Computational Modelling of Graphene Materials.

Molecular Dynamics Simulations of Graphene and Related Materials: Graphene—a material that is currently drawing huge scientific and technological interest—is an allotrope of carbon with a unique two-dimensional structure formed by hexagonal honeycomb lattice. It has some very unique physical, opto-electronic and mechanical properties. For instance, its tensile strength is 150 times that of steel.

In these projects, using molecular dynamics simulations, we will aim to study how the atomic-level structural details control the microscopic physical and mechanical behaviour of graphene and related materials. These simulations will range from a few hundred atoms to thousands of the atoms at a time and will be performed on high-performance parallel computing infrastructure.