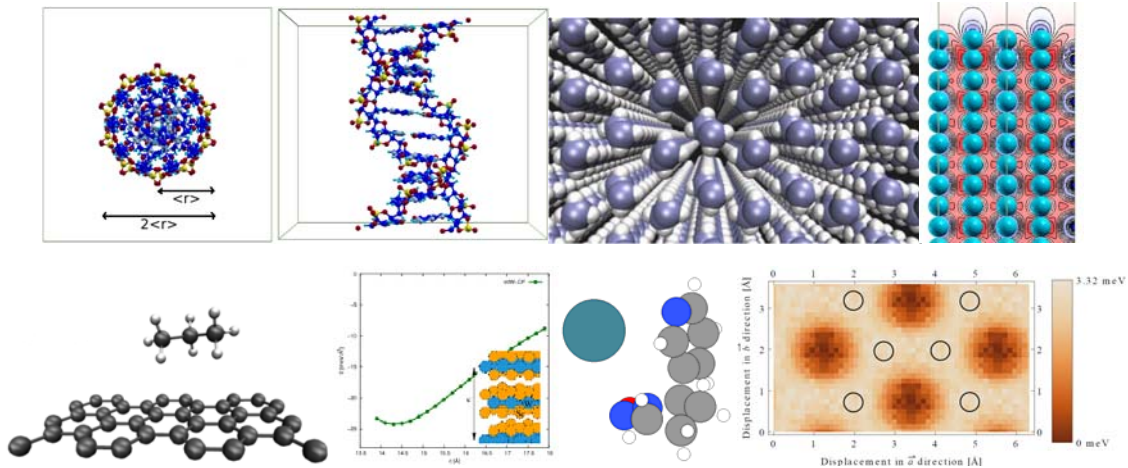


Materials theory on the atomic scale



Most of the world around us consists of materials in one or the other form. Much research depends on knowing the properties of materials, for example adsorption energies on surfaces, conformations of molecules under various conditions, or the charge transport in electronic components.

Materials theory has a set of modern efficient and accurate methods that are being used to evaluate, predict and analyze the properties of almost any material, from hard metal surfaces to gas phase organic molecules.

We use the method density functional theory (DFT) for materials calculations in a wide range of areas, for example to study pollutant molecules in carbon filters, the oxidation of magnesium surfaces, or the structure of bits of DNA. The scope is wide, and the possible directions for a master's projects are numerous. ***I welcome you to come to talk with me (contact details below) about your interests and ideas and together we can find and define a project that suits your background and interests.***

Target group for the project: This is suited for students in the Chalmers nano, materials, or physics-related programmes, it may also fit students with a chemistry background. The project is also open for GU students with a similar background.

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