# Computational materials design and characterisation for functional materials

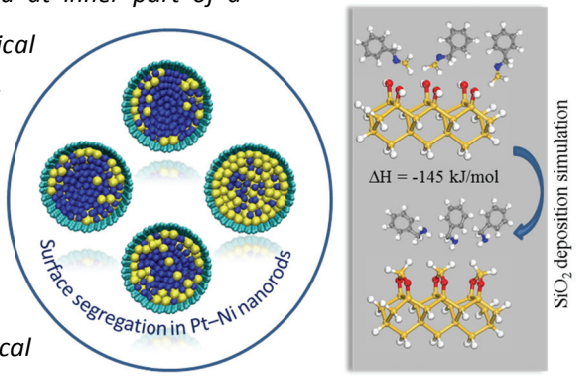
**D**ensity functional theory is a modeling and simulation tool to allow researchers in materials science and chemistry to predict and understand the relationships of a material's atomic and molecular structure with its properties and behavior. In NAFUMA we target better performing materials; photovoltaics, catalysts, thin films/coatings, microporous materials, metals and alloys, batteries, sensors, multiferroics, nanoparticles and surfaces, etc. Modeling allows us to develop new, better performing, and more cost effective materials faster and more efficiently than with synthesis, tests and experimentation alone. The project will involve extensive use of advanced computational tools available in our group and the simulations are executed in the supercomputer facility available in Norway. The theoretical studies may be combined with experimental work if desired.

Examples of this:

- How can we alter the properties of materials by nanoengineering?
- How to find fast Li/Na conductive electrode materials by theoretical simulation?
- Why does chemical composition at a surface differ from the inner part of the material?
- Identify active precursors for atomic layer deposition and their reactivity at the surfaces
- Explore the new intermediate band gap material for PV applications
- How is the electronic structure of a material modified by chemical substitutions or pressure?

What you may learn:

- *How to use the DFT to find/characterize functional materials*
- *Combine DFT along with classical molecular dynamics*
- *Identify chemical composition at surfaces and at inner part of a system; or become able to model chemical reactions and pathway, diffusion or molecular absorption and transition states*
- *Become able to predict stability and performance of known and new compounds; e.g. new electrode materials for Na- batteries*
- *Deeper insight in defect and thermodynamical stability of materials*
- *Become a key part of the NAFUMA group and work closely with the experimentalists*




**Type of project**: Computer modelling in materials science
**Research group**: NAFUMA
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