

## **Biplab Sanyal**

### **Bio**

Docent (Asst. Professor) at the University of Uppsala, Sweden. In the department of Physics and Material Sciences.

PhD in Physics, condensed matter theory, from Jadavpur University, Calcutta, India.

### **Quantum mechanical modeling of advanced materials**

Understanding of the properties of materials in an atomic scale is an important issue in order to develop new materials for a better technology. This becomes particularly important for materials at a nano-scale where quantum mechanical interactions dominate the physical properties. I will demonstrate a few important examples of materials research where first-principles density functional theory has been employed to understand the physics. These examples include magnetic interactions between bio-molecules and magnetic substrates (ref. 1), complex interactions in diluted magnetic semiconductors and the effects of defects in graphene.

#### **References**

Wende et al., Nature Materials 6, 516 (2007).

The intended mode of cooperation will be to identify and collaborate on interesting materials with novel properties, development of methods suitable for the calculations of specific properties, multiscale modeling techniques and different numerical aspects to increase the efficiency of softwares used for materials modeling.