

# Warwick Chemistry Departmental Seminar



**Professor Bo Iversen**

Aarhus University

**Thursday 6 December**

**4.00 pm, Physics Lecture Theatre, Science Concourse**

## **“Chemical bonding in layered thermoelectric materials”**

Layered (2D) materials exhibit a variety of extraordinary properties, and recent focus has included topological insulators, electrode materials, monolayers, hetero structures – and thermoelectrics. It is generally assumed that layered materials exhibit strongly anisotropic properties, but the properties are rarely discussed in direct relation to the specific chemical bonding characteristics of the solid. Using advanced crystallographic analysis including charge density modelling as well as ab initio theoretical calculations we have studied the crystal structures and chemical bonding of a range of important layered thermoelectric materials including  $\text{Cu}_2\text{Se}$ ,  $\text{Mg}_3\text{Sb}_2$ ,  $\text{SnS}_2$  and  $\text{TiS}_2$ .