

## School of Chemistry

### Aims and Objectives: Session 2023-2024, Semester 2

#### Module CH3712: Quantum Theory of Atoms, Molecules and Solids

**Course Title:** Advanced Solid State Chemistry

**Duration:** 7 hours

**Lecturer:** Professor F. D. Morrison

**Aims:** To be familiar with the structures of several complex solids including perovskites and spinels. To understand the origin of non-stoichiometry in solids and its consequences for properties. To understand band theory of solids in the context of both “nearly-free” and “tight-binding” electron models. To understand how the electronic structure of transition metal solids such as TiO and NiO may be described by extending the principles by which electronic structure of transition metal coordination complexes are described. To appreciate that in the solid state d-electrons can be localised or delocalised and to understand the forces at work in determining which of these states is adopted. To understand the basic types of magnetic ordering and why these arise.

**Objectives:**

1. To be in a position to describe the structures of several important solids including perovskites and spinels.
2. To understand how solids may exhibit non-stoichiometry and the effect this can have on their properties. To understand how extended defects can form in ionic solids.
3. To understand the origin of band formation in solids in the context of both “nearly-free” and “tight-binding” electron models.
4. To understand how the electronic structure of transition metal solids such as TiO and NiO may be described by extending the “tight-binding” description used for transition metal complexes.
5. To appreciate that d-electrons and transition metal solids can be localised or delocalised and to understand the competing forces, which determine whether in any given material the electrons will be localised or delocalised. Furthermore, to appreciate the relevance of this to the electronic conductivity of the compounds.
6. To understand the factors which drive ferromagnetic and antiferromagnetic ordering in solids.