Materials Chemistry
(updated March 2015)

Lecture Content

1. Introduction and close packed structures (Prof. Brendan Kennedy)
   - Course outline
   - Revision of Chem 2

2. Interaction of X-rays and electrons with matter (Prof. Brendan Kennedy)
   - X-ray diffraction
   - Scattering spectroscopy vs diffraction

3. Diffraction 1 – Symmetry (Prof. Brendan Kennedy)
   - Space groups

4. Diffraction 2 – Miller indices (Prof. Brendan Kennedy)
   - Labeling Miller indices
   - Bragg diffraction

5. Diffraction 3 - Thermal Expansion (Prof. Brendan Kennedy)

6. Allied methods. XPS and XANES (Prof. Brendan Kennedy)
   - Case study LaMnO$_3$

   - Case study CdVO$_3$ and CdTiO$_3$:
     - One composition difference structures. High pressure vs ambient pressure

8. Neutron and synchrotron diffraction (Prof. Brendan Kennedy)
   - What is a synchrotron?
   - Why use neutron diffraction?
   - Comparison of X-ray and neutron diffraction
9. Bonding - I (A/Prof. Chris Ling)
Ionic vs covalent bonding in solids:
- Effective ionic radii
- Lattice energy of ionic crystals
- Coordination spheres and Madelung constants
- Covalency as an explanation of non-close-packed structures
- Non-bonding electron effects
- Bond valence sums

10. Bonding - II (A/Prof. Chris Ling)
Metallic bonding:
- Tight binding approximation
- Band structures
- 1-D, 2-D and 3-D conductors
- Electron localization (Mott-Hubbard insulators)
- Electronic bonding in inorganic solids
- Doped semiconductors
- Thermoelectricity
- Conductivity/resistivity and carrier mobility
- Temperature dependence of conduction in metals/semiconductors/insulators

11. Magnetism - I (A/Prof. Chris Ling)
The origin of magnetism in materials:
- The magnetic moment of an atom
- Crystal-field effects on magnetism in materials
Measuring and classifying magnetism in materials:
- Diamagnetism
- Paramagnetism
- Ferromagnetism
- Antiferromagnetism
- Ferrimagnetism

12. Magnetism - II (A/Prof. Chris Ling)
- Orbital ordering
- Magnetostriction
- Magnetoresistance
- Magnetic neutron scattering
13. **Superconductivity** *(A/Prof. Chris Ling)*

**History:**
- Conventional superconductors from Hg to Nb$_3$Ge
- Unconventional superconductors from La$_{1.8}$Ba$_{0.2}$CuO$_4$ to Hg-1223

**Properties:**
- Zero resistance (BCS theory)
- Superdiamagnetism (Meissner effect), vortex lattices (types I and II)
- Applications (conductors, electromagnets, SQUIDs, levitation ...)

**Structural, chemical, and electronic themes:**
- Hole/electron doping of half-filled bands
- Layered structures (charge reservoir layers)

14. **Silicates - I** *(A/Prof. Chris Ling)*

Silicate anions: the building blocks:
- The natural forms of silica (SiO$_2$): quartz, glass, cristobalite etc
- Breaking silica down into building blocks: silicate anions clays
- Structure and bonding
- Intercalation properties
- Modifications (pillaring)

15. **Silicates - II** *(A/Prof. Chris Ling)*

Zeolites:
- Structure and building blocks
- Synthesis and structural properties
- Chemical and catalytic properties
- Post-synthesis modifications (ion exchange)

Macroporous materials:
- Synthesis, properties, and characterization
- Non-silicate zeotypes

16. **Fuel cells** *(A/Prof. Siggi Schmid)*

- Point defects
- Extended defects
- Solid solutions
- Phase diagrams
- Ionic conductivity
- Fuel cells
17. Batteries (A/Prof. Siggi Schmid)
   - Chemical energy storage
   - Types of batteries
   - Rechargeable Li ion batteries
   - Intercalation battery materials

18. Ferroric materials I (A/Prof. Siggi Schmid)
   - Ferroelectricity
   - Ferroelectric materials
   - Symmetry requirements

19. Ferroric materials II (A/Prof. Siggi Schmid)
   - Pyroelectricity
   - Piezoelectricity
   - Symmetry requirements

20. Shape memory alloys (A/Prof. Siggi Schmid)
   - Metal structures
   - Alloys
   - Properties
   - Shape memory

21. Stabilised zirconia (A/Prof. Siggi Schmid)
   - Mechanical properties
   - Tough ceramics
   - 2 phase mixtures

22. Non-classical crystallography (A/Prof. Siggi Schmid)
   - Classical crystallography
   - Long-range order
   - Short-range order
   - Aperiodicity