Graph Theory with Applications in Chemistry I
(Chair/Président: **Patrick Fowler** (University of Sheffield)
Org: **Patrick Fowler** (University of Sheffield) and/et **Wendy Myrvold** (University of Victoria))

MATTHIAS ERNZERHOF, University of Montreal
The zero-voltage conductance of nano-graphenes: Simple rules and

Zero-dimensional graphenes, or nano-graphenes (NGs), are fragments of graphene with a finite number of hexagons, and form a subset of the polycyclic aromatic hydrocarbons. We develop a simple theory for ballistic electron transport through NGs which combines electronic structure theory of graphene, intuitive methods for calculation of molecular conductance, and chemical concepts such as Kekulé structures. This theory enables analysis of relations between structure and conductance. General formulas and rules for zero-voltage conductance as a function of contact positions are derived. These require at most simple paper and pencil calculations in applications to systems containing tens of carbon atoms.

PATRICK W FOWLER, University of Sheffield
Conjugated circuits, currents in benzenoids and equiaromaticity

Benzenoids are simple planar 2-connected graphs embedded in the plane with hexagonal internal faces, internal vertices of degree 3 and external vertices of degree 2 or 3. Cycle C in graph G is a conjugated circuit if both G and G-C have perfect matchings. Chemical aromaticity implies that a molecule supports magnetically induced ring currents. Models for these currents are often based on conjugated-circuit contributions. We identify *equiaromatic* benzenoids, where corresponding rings support equal currents, with implications for molecular properties and connections with Fibonacci and Lucas numbers.

*Joint work with Sam Cotton, Dan Jenkinson, Wendy Myrvold and William Bird

WENDY MYRVOLD, University of Victoria
Models of Current Density Maps of Benzenoids

Benzenoids correspond to embeddings of 2-connected planar graphs with hexagonal internal faces, external vertices of degree 2 or 3, and all others of degree 3. A $conjugated\ circuit$ of graph G is a cycle C such that $G - C$ has a perfect matching. Conjugated-circuit models for magnetically induced currents in benzenoids represent them by direction and magnitude for each edge, as do Hückel-London models. Ab initio and Pseudo-π computations allow through-space flow (represented on a grid). The goal is to compare (and improve) the simple models.

*Joint work with William Bird, Matthew Imrie and Patrick Fowler.

BARRY T PICKUP, University of Sheffield
Effects of Pauli blockade on single-molecule conduction

The conduction of electrons through devices made of single molecules has been well studied using Hückel theory in a one-electron picture. The introduction of many-electron effects into this model introduces dramatic changes in conductivity which are simply understood in terms of a 'Pauli blockade' effect, in which electrons are prevented from travelling through orbitals which are already occupied. This talk provides simple analytical expressions derived from spectral decomposition of characteristic polynomials, within the essentially graph theoretical source-sink potential method.

IRENE SCIRIHA, University of Malta
Molecular Graphs with Analogous Conducting Connections

In the graph-theoretical Source and Sink Potential model, a molecule is either an insulator or a conductor for electrons with energy zero. Of particular interest are two classes of graphs with analogous vertex pairs, i.e., the same behaviour for any two-vertex connection. These are *uniform-core* (insulating for all two-vertex connections) and *nuciferous* graphs, which conduct for all two-vertex connections. A graph G in the first class reaches the minimum possible nullity when any two distinct connecting vertices are deleted. In the second class, the nullity reaches one, the maximum possible, when any vertex is deleted.