Graph theory for molecular currents: conduction and aromaticity

Patrick W Fowler
University of Sheffield

Abstract

Molecules are not graphs, but a surprising variety of molecular properties can be predicted and rationalised using graph-theoretical methods and simple physical models. In turn, the physical models raise mathematical questions and motivate some conjectures. This talk will focus on the currents that are induced in molecules by an external magnetic field (ring currents) or the application of a potential difference across two leads (ballistic molecular conduction).

Selection rules based on symmetry and graph theory predict the sense of the ring current (distinguishing aromatic and antiaromatic molecules) and the presence (or absence) of conduction at the Fermi level. Special classes of molecules/graphs are of interest: e.g. chemical graphs, omni-conductors, omni-insulators, nut graphs. Nut graphs are singular, have nullity one, and have a full kernel eigenvector. They figure prominently in qualitative theories of reactivity, stability and molecular conduction. Orders and degree sequences of chemical nut graphs have been established.