
PATRICK FOWLER, University of Sheffield

Currents in molecules

Two applications of graph theory to determination of electron flow in molecules are presented. Ballistic currents, driven through a molecule by a potential difference, are described in terms of a transmission function based on characteristic polynomials of the molecular graph and three vertex-deleted subgraphs. Ring currents, flowing in closed loops within a molecule and driven by an applied magnetic field, are described in terms of nodal characteristics of adjacency eigenvectors of the molecular graph.