

Some current work on currents

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Currents within and through molecules are of interest in chemistry and physics for several reasons. For example, circulations induced by a magnetic field (ring currents) are related to experimental NMR signatures of aromatic molecules and the vexed question of how to define aromaticity. On the other hand, ballistic currents induced by potential differences are related to molecular electronics.

This talk will describe some of our recent work on modelling molecular currents at various levels of theory, with emphasis on the construction of very simplest models, cast in terms of chemical concepts.