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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.