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Bond resistances in molecular junctions ANNA PAINELLI, Universita' di Parma & INSTM UdR Parma — The description of molecular contacts is one of the hardest problems in modeling molecular junctions. In common approaches macroscopic leads ensure a finite potential drop and hence a driving force for the current. Recently, a different strategy is emerging where a steady-state DC current is forced in the molecule, by making resort to Lagrange multipliers, or by drawing a magnetic flux through the molecule. The strategy is promising, but two main problems remain to be solved: (1) the calculation of the potential drop needed to sustain the current, and (2) the definition of the potential profile along the molecule. Here the Joule law is used to evaluate the potential drop from the electrical power spent on the molecule, and continuity constraints for steady-state DC current are implemented to get information on the potential profile. Borrowing powerful concepts from the field of molecular spectroscopy, emphasis is put on the molecule, while clamping information about contacts in the molecular relaxation matrix. The molecule is described in a real-space approach, leading to a suggestive analogy between the molecule and an electrical circuit where resistances are associated with chemical bonds.

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