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The Role of Symmetry in Molecular Electronic Conduction

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The Greens Function Density-Functional Tight-Binding (gDFTB) method is applied to determine the role that molecular symmetry in single-molecule conductivity. Both coherent elastic electron transport and inelastic electron-tunnelling spectroscopy (IETS) are considered. Symmetry becomes manifest in various ways: through the molecular point-group symmetry of the conducting molecule (D_{2h} for chemisorbed benzenedithiol between two gold electrodes), through the conductance point-group symmetry displayed by the gDFTB equations (this embodies junction asymmetry and may be very low and nominally non-existent), and through an approximate molecular-conductance point group (C_{2v} for chemisorbed benzenedithiol). Indeed, the conductivities for a range of relevant problems are well approximated using the restriction of molecular-conductance point-group. This allows the complex transmission curves calculated by many research groups to be dramatically simplified and partitioned into symmetry-depicted channels. Means are introduced that isolate a very small number of component channels describing different aspects of single-molecule conductivity: input junction channels, through-molecule channels, and output-junction channels. For elastic transport, all through-molecule channels are totally symmetric and hence a rigorous selection rule appears that transport is allowed involving only input-junction and output-junction channels of the same symmetry. However, for IETS, the through-molecule channels have the symmetry of the scattering molecular vibration and hence the input-junction and output-junction channel symmetries may vary. In general, just one channel is expected to dominate the junctions, leading to the IETS propensity rule that totally symmetric transitions are the most intense ones. Simple physical pictures are presented showing the input, vibrational scattering, and output channels for IETS, leading to predictions of how this effect can be controlled chemically.