Engineering Quantum Properties of Molecular Circuits with Chemistry

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I will describe my lab's recent progress in demonstrating and controlling quantum phenomena in single molecule junctions. We demonstrate that synthetic modifications can be leveraged to create functionality in such structures, with potential in quantum sensing, switching and high conductance of topological electronic states in molecules. I will describe in more detail the high conductance of topological insulator molecular wires we observe and the expanded 1D Su-Schriefer-Heeger model we developed to explain our observations. Specifically, I will show that we achieve, at room temperature, conductance enhancements over two orders of magnitude in single molecule circuits formed with polycyclic benzoquinoidal (BQ_n) diradicals upon increasing molecular length by ~5 Å. We find that this extreme and atypical anti-ohmic conductance enhancement at longer molecular lengths is due to the diradical character of the molecules, which can be described as a topologically non-trivial electronic state. We adapt the 1D-SSH model originally developed to examine electronic topological order in linear carbon chains to the polycyclic systems studied here and find that it captures the anti-ohmic trends in this molecular series. The mechanism of conductance enhancement with length is revealed to be constructive quantum interference (CQI) between the frontier orbitals with non-trivial topology, which is present in acene-like, but not in linear, molecular systems. Importantly, we predict computationally and measure experimentally that anti-ohmic trends can be engineered through synthetic adjustments of the diradical character of the acene-like molecules. Overall, we achieve an experimentally unprecedented anti-ohmic enhancement and mechanistic insight into electronic transport in a class of materials that we identify here as promising candidates for creating highly conductive and tunable nanoscale wires.