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Unusual Conductance in Cumulene Molecular Wires JARIYANEE PRASONGKIT, Condensed Matter Theory Group, Dept. of Physics and Materials Science, Uppsala University, Sweden, ANTON GRIGORIEV, CMT Group, Uppsala, GÖRAN WENDIN , Department of Microtechnology and Nanoscience, Chalmers University of Technology, Gothenburg, Sweden, RAJEEV AHUJA, CMT Group, Uppsala; Applied Materials Physics, Dept. of Materials and Engineering, Royal Institute of Technology (KTH), Stockholm, Sweden — We report current-voltage curves and conductance of cumulene molecular wire suspended between Au(111) surfaces via thiolate bonds with full self-consistent *ab initio* calculation under external bias. The conductance of cumulene wires shows oscillatory behavior depending on the number of carbon atoms. Among all conjugated oligomers, we find that odd-number cumulene wires yield the highest conductance and present ballistic-like transport behavior. The reason has been traced to two factors: high density of state at the Fermi level, and the alignment of molecular orbital closed to Fermi level. Since the conductance depends weakly on applied bias, and the current voltage characteristic is linear under bias region -0.9 to 0.9 V, odd-number cumulene wire is a possible candidate as a near- perfect, ballistic one-dimensional molecular wire.

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