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Understanding the Role of Direct Au-C Links to Electrodes in Single Molecule Junctions[1] HECTOR VAZQUEZ, JONATHAN WIDAWSKY, ZHANG-LING CHENG, SEVERIN SCHNEEBELI, RACHID SKOUTA, RONALD BRESLOW, MARK S. HYBERTSEN, LATHA VENKATARAMAN — Recent experiments have shown that use of tri-methyl tin (SnMe3) link groups results in the formation of alkane single molecule junctions with measured conductance $\sim$100 times higher than found for any other link group previously used. Further evidence points to the in-situ formation of direct Au-C bonds to the electrode. In this work we use Density-Functional Theory based calculations to study the formation and structure of junctions based on direct Au-C link bonds. Transport calculations based on Non-Equilibrium Green's Functions for benzene and alkane molecules anchored through Au-C bonds show that the alkane backbone couples more strongly to the leads, resulting in a higher transmission as compared with other link groups. In the case of benzene, however, transport is primarily through the σ system, yielding a smaller conductance increase. Finally, we discuss corrections to the position of molecular resonances found in the DFT-based calculations and the implications for conductance.

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Hector Vazquez
Columbia University

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