



How Low Can We Go? The Search For Quantum Interference Based Single-Molecule Insulators

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While there has been significant focus on making high-conductance molecular wires, it is equally challenging to make extremely low conductance systems. Here we present some of our efforts to find highly insulating molecules. We have found the first molecule with clear suppression of the single-molecule conductance due to σ -interference in the form of a functionalized bicyclo[2.2.2]octasilane¹. The interference effects in this system are so significant that our calculations show the central unit is more insulating than a vacuum gap of the same dimensions. Through an extensive investigation of a family of cyclic and bicyclic silanes² we show that their transport properties can largely be understood by considering these otherwise complex molecules as constrained linear systems. From a high-throughput screening study³ varying the constituent atoms between carbon, silicon, and germanium, we know that majority of the molecules in the bicyclo[2.2.2]octane class are likely highly insulating. Finally, we have recently discovered that substituents play a major role in controlling interference and side-groups previously thought to be unimportant can be critical for the appearance of significant destructive interference⁴.

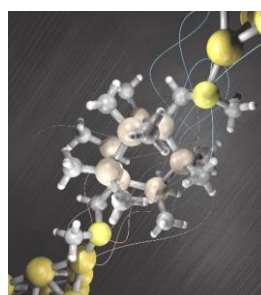


Figure 1. A ball and stick model of the bicyclo[2.2.2]octasilane based system with a central insulating unit that was shown to be more insulating than a vacuum gap of the same dimensions.¹

References: 1. Garner, M. H.; Li, H.; Chen, Y.; Su, T. A.; Shangquan, Z.; Paley, D. W.; Liu, T.; Ng, F.; Li, H.; Xiao, S.; Nuckolls, C.; Venkataraman, L.; Solomon, G.C. Comprehensive suppression of single-molecule conductance using destructive σ -interference *Nature* **2018**, 558, 415-419. 2. Li, H.; Garner, M. H.; Shangquan, Z.; Chen, Y.; Zheng, Q.; Su, T.; Neupane, M.; Liu, T.; Steigerwald, M.; Ng, F.; Nuckolls, C.; Xiao, S.; Solomon, G.C.; Venkataraman, L. Large Variations in Single Molecule Conductance of Cyclic and Bicyclic Silanes *J. Am. Chem. Soc.*, **2018**, 140 (44), 15080–15088. 3. Garner, M.H.; Koerstz, M.; Jensen, J.H.; Solomon, G.C.; The Bicyclo[2.2.2]octane Motif: A Class of Saturated Group 14 Quantum Interference Based Single-Molecule Insulators *J. Phys. Chem. Lett.*, **2018** 9(24), 6941-6947. 4. Garner, M.H.; Li, H.; Neupane, M.; Zou, Q.; Liu, T.; Su, T. A.; Shangquan, Z.; Paley, D. W.; Ng, F.; Xiao, S.; Nuckolls, C.; Venkataraman, L.; Solomon, G. C. *J. Am. Chem. Soc.* **2019**, in press.

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