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Conformations of cyclic silanes control molecular junction conductance[1] HAIXING LI, Columbia Univ, MARC GARNER, University of Copenhagen, ZHICHUN SHANGGUANG, QIANWEN ZHENG, YAN CHEN, Shanghai Normal University, TIMOTHY SU, MADHAV NEUPANE, MICHAEL STEIGERWALD, Columbia University, SHENGXIONG XIAO, Shanghai Normal University, COLIN NUCKOLLS, Columbia University, GEMMA SOLOMON, University of Copenhagen, LATHA VENKATARAMAN, Columbia University — We examine the impact of ring conformation on the charge transport characteristics of cyclic silicon structures bound to gold electrodes in single molecule junctions. We investigate the conductance properties of cyclic silanes using both the scanning tunneling microscope based break junction technique and density functional theory based ab initio calculations. In contrast with the linear ones, these cyclic silanes yield lower conductance values; calculations reveal that the constrained dihedral geometries occurring within the ring are suboptimal for σ-orbital delocalization, and therefore, conductance. Due to the weakened σ-conjugation in the molecule, through-space interactions are found to contribute significantly to the conductance. This work details the vast conformational flexibility in cyclic silanes and the tremendous impact it has on controlling conductance.

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