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Controlling Current Flow Through Molecules With Electric Fields Emanating From Nearby Molecules: Theory and Experiment[1] G. KIRCZENOW, Simon Fraser U., P. G. PIVA, R. A. WOLKOW, NINT and U. of Alberta — We show that electrical conduction through molecules can be strongly modulated by electric fields of nearby polar molecules. We study 1D organic heterostructures consisting of contiguous lines of CF_3- and OCH_3-styrene molecules on H-terminated Si(100). For suitable alignment of the OCH_3 groups in the molecular chain, their combined electric fields are shown by density functional calculations to give rise to potential profiles along the OCH_3-styrene chain that result in strongly enhanced conduction through molecules near the CF_3-styrene/OCH_3-styrene heterojunction for moderately low negative substrate bias, as is observed by STM. Under similar bias, dipoles associated with CF_3 groups are found in both theory and experiment to depress transport in the underlying Si. Under positive substrate bias, simulations suggest that the structural and electrostatic properties of CF_3-styrene molecules may lead to more sharply localized conduction enhancement near the heterojunction. Thus choice of substituents, their attachment site on the host styrene molecules on Si and the orientations of the molecular dipoles and multipoles provide a means of differentially tuning transport on the molecular scale.

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