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Electron Transport Through Molecules: Gate Induced Polarization and Potential Shift SAN-HUANG KE, HAROLD U. BARANGER, WEITAO YANG, Duke University — We analyze the effect of a gate on the conductance of molecules by separately evaluating the gate-induced polarization and the potential shift of the molecule relative to the leads. The calculations use *ab initio* density functional theory combined with a Green function method for electron transport. For a general view, we study several systems: (1) atomic chains of C or Al sandwiched between Al electrodes, (2) a benzene molecule between Au leads, and (3) (9,0) and (5,5) carbon nanotubes. We find that the polarization effect is small because of screening. The effect of the potential shift is significant, providing a mechanism for single-molecule transistors. This work was supported in part by the NSF (DMR-0103003).

San-Huang Ke
Duke University

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