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Self-Consistent Non-Equilibrium Green's Function Considerations in STM Height Models Applied to Si(100) K.H. BEVAN, Purdue University, F. ZAHID, McGill University, D. KIENLE, Purdue University, H. GUO, McGill University — In this study we report on the self-consistent non-equilibrium potential drop between Si(100) and a scanning tunneling microscope (STM) tip. It is found to play a role in the height characteristics of adsorbed hydrocarbons in conjunction with the silicon band gap. Results are reported for styrene against a hydrogen passivated Si(100) background. The potential drop is found to reduce the effective STM height of styrene by shifting molecular levels. Calculations are performed within density functional theory (DFT) under both the self-consistent and non-self consistent non-equilibrium Green's function (NEGF) formalism. Tunneling current distance dependence is captured by an ab-initio basis via free pseudopotential eigenstates benchmarked for clean metallic surfaces. The resulting trends indicate that participation of an applied bias potential profile in measured STM surface heights should not be limited to Si(100).

Kirk H. Bevan
Purdue University

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