*Poster*

**FIRST-PRINCIPLES ANALYSIS OF STM IMAGE HEIGHTS ON SI(100)**

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We report on theoretical investigations of STM image heights on Si(100). Calculations are performed using density functional theory (DFT) within the Keldysh non-equilibrium Green's function (NEGF) formalism. The non-equilibrium potential drop between Si(100) and a scanning tunneling microscope (STM) tip is determined self-consistently. This potential drop is found to play an important role in the calculated image height characteristics of adsorbed hydrocarbons, by lowering the vacuum barrier and shifting molecular levels.
Numerical data collected for image heights of styrene against a hydrogen passivated Si(100) background are found to agree quantitatively with the corresponding experimental results. We also present a comparison between results obtained by the NEGF-DFT formalism and the Tersoff-Hamann approximation, showing that non-equilibrium analysis can be important in the study of STM image heights of molecules.