CHARGE STATE OF DANGLING BONDS ON Si-H SURFACE UNDER STM IMAGING

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After termination with hydrogen, a silicon surface usually naturally retains a certain density of dangling bonds (DBs). On an undoped sample, DBs are occupied by a single electron, but on n-type samples, DBs can become doubly-occupied, yielding a net negative charge – this acceptor level is located around mid-gap for Si. Charge will accumulate on the surface until the induced potential shifts the surface DB acceptor level to equal the Fermi level, bending the bands up. The introduction of a STM tip perturbs the system and tends to either attract or repel the electrons occupying the surface, screening the potential of the tip. This has the effect of pinning the Fermi level near the DB acceptor level over a certain range of tip voltages, which depends on surface DB concentration and dopant levels.

Semi-classical calculations using the finite element method are presented that solve this system in general, allowing spatially varying dopant densities, different tip sizes, DB acceptor levels and surface DB concentrations. We show how the presence of a tip affects the average DB charge density, and present experimental STM images confirming the expected effect [1]. These images additionally show how the charge of a DB locally affects imaging over < 1 nm length scales, shifting molecular levels in nearby molecular lines. The calculations presented are electrostatic and assume negligible current flowing through the STM tip – future extensions to the calculations will include steady-state conditions with non-zero current.

References

[1] Piva, P. et al., Nature, *In press.*