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Theory of Scanning Tunneling Microscopy of Dangling Bonds on Silicon Surfaces LUCIAN LIVADARU, University of Alberta, JASON PITTERS, NINT, ROBERT WOLKOW, University of Alberta/NINT — Silicon surface dangling bonds (DBs) are electronic gap states with eigenenergy close to the middle of the bandgap of bulk silicon and can be explored as quantum dots. During exploratory fabrication and characterization of DB-structures on H-Si(100) surfaces, scanning tunneling microscopy (STM) imaging showed sharp halo-like features around single DBs that cannot be explained by the standard STM theory. Halo appearance varies with sample doping level and imaging conditions (sample bias and current). Here we investigate the nature of such features in the STM imaging of DBs. We propose a theory of image formation based on non-equilibrium charge transfer balance (via elastic and inelastic channels), from the STM tip to DB on one hand, and from DB to bulk Si on the other. For empty-state imaging mode, in the immediate proximity of a DB ($<1\text{nm}$) tip-induced band bending shifts the DB-level to a value between the Fermi levels of the STM tip and of the sample. Consequently, a steady-state of charge flow is established through the DB state, which dictates the time-average amount of charge on the DB. This in turn affects the total STM current in that proximity leading to the appearance of a halo.

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