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Charge-State Dependent Hydrogen Diffusion on Silicon (001) OLIVER WARSCHKOW, University of Sydney — The diffusion of hydrogen atoms is relevant to a number of chemical and technological processes of the silicon (001) surface. These include the dissociative adsorption of molecules, the growth of overlayers by chemical vapor deposition (CVD), and the directed atomic-scale functionalization of the surface by scanning tunnelling microscopy (STM) lithography. The basic inter- and intradimer shift reactions of hydrogen are well studied, and activation energies of respectively 1.7 eV and between 1.0 and 1.4 eV are commonly cited. In this presentation, I will pose and discuss two questions: (1) Are single energy barriers adequate to describe H-shift reactions on silicon, and (2) are STM measurements of H-diffusion truly representative for hydrogen desorption in the absence an STM tip? These questions warrant examination because hydrogen adatoms on Si(001) are known to adopt a variety of charge states depending on factors such as the doping level of the silicon substrate, the defect density on the surface, or the presence of an STM tip. High-level density functional calculations are reported to shed some clarity on these questions.

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