

Water-induced point defects on the dimerized Si(001) surface*

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Perhaps, silicon (001) wafer is the most studied and best understood material for its extensive utilization in semiconductor electronic device industry. Through decades-long studies employing both experimental and theoretical means, the pristine surface structure (the so-called dimerization reconstruction) and its electronic structure has been fully accounted for. More complicated phenomena such as surface point defects and the adsorption of heterogeneous molecules seems to have been well understood. However, with the advancement of nano-sciences and atomic scale probes like scanning tunneling microscopy (STM), apparently well-understood processes start to reveal intriguing phenomena that questions previous knowledge. In this lecture, we demonstrate that a significant part of the presumed intrinsic defects on Si(001) are dissociatively adsorbed water molecules by employing the STM measurements and the first-principles calculations.

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