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Temperature dependent adsorption and dissociation of water molecules on the Si(001)-(2 × 1) surface JA-YONG KOO, Korea Research Institute of Standards and Science, YONG-SUNG KIM, HANCHUL KIM, SANG-YONG YU — The dissociative adsorption of water molecules on the Si(001)-(2 × 1) surface was studied up to 850 K by scanning tunneling microscopy (STM). A water molecule is dissociated into on-dimer (OD) and inter-dimer (ID) configurations and the population ratio n_{ID}/n_{OD} changes from ~ 5 at room temperature to ~ 0.5 above 500 K. A quantitative analysis was made by considering the flipping motion of Si dimers to overcome the discrepancy between the experiment and theoretical estimations from the model of simple energy barrier. The flipping motion of Si dimers plays a dominant role in the dissociation of water molecules on the Si (001)-(2 × 1) surface.

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