[총회초청 I]

Dynamics of Hydrogen on Si(100)

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In this talk we discuss the dynamics of hydrogen on the Si(100)-2x1 surface. At room temperature the sticking coefficient for molecular hydrogen on this surface is less than 10sup-12. However, hydrogen molecules desorbing from the surface do not have an excess of energy, suggesting at best a small barrier on the exit channel. These observations have led to speculation about the validity of detailed balance in this system. Here we show that this discrepancy can be explained by considering both the surface-molecule co-ordinate and that associated with the Si-Si dimer bond tiltangle. By preparing the surface dimers with a specific tiltangle we demonstrate that the barrier to adsorption is a function of this angle and that the sticking coefficient dramatically increase for certain angles. The adsorption-desorption dynamics can then be described in terms of a common potential energy hypersurface involving both of these co-ordinates. The implications of these observations are also discussed.

The dynamics of adsorbed hydrogen atoms on the Si(100) surface is also described. Paired dangling bonds produced following recombinative hydrogen desorption are mobile at elevated temperatures. Pairs of dangling bonds are observed to dissociate, diffuse, and ultimately recombine. At sufficiently elevated temperatures dangling bond exchange reactions are observed. These data are analyzed in terms of an attractive zone and an effective binding interaction between dangling bonds. Insights that this provides into the nature of surface defects and the localized chemistry that occurs on this surface, are also discussed.