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First-principles Study of the Structure and Growth Mechanism of Allyl Alcohol Lines on the H-terminated Si(001)

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Using first-principles density-functional calculations, we investigate the chain reaction mechanism of allyl alcohol (ALA) molecules on the H-terminated Si(001)-2×1 surface. Recently, it was reported [1] that allyl mercaptan (ALM) molecules show a self-directed line growth across the dimer rows through a chain reaction involving several reaction processes: (i) The created radical at the C atom is transferred to the S atom, (ii) the resulting S-centered radical easily abstracts an H atom from the neighboring dimer row, and (iii) the generated S-H group further reacts with the neighboring dimer row to produce the Si-S bond on the neighboring dimer row, accompanying the associative desorption of H2. This H2-desorption process creates a new DB on the neighboring dimer row, setting off the chain reaction across the dimer rows. In the present study, we find that although the structure of ALA with −OH functional is analogous to that of ALM with −SH functional, ALA and ALM lines show a difference in their growth direction. We predict that ALA undergoes the chain reaction to show a line growth along the dimer row, contrasting with the ALM line growth across the Si dimer rows. Our analysis shows that the different growth direction of ALA is due to the strong instability of oxygen radical intermediate, which prevents from growing across the dimer rows. Thus, we demonstrate that the stability of the radical intermediate plays a crucial role in determining the direction of molecular line growth.

[1] J.-H. Choi and J.-H. Cho, Phys. Rev. Lett. 102, 166102 (2009).

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