

New Self-Directed Growth Mechanism of Molecular Lines across the Dimer Rows on H-terminated Si(001) Surface

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We present theoretical investigations of the self-assembled growth of one-dimensional (1D) molecular lines directed across the dimer rows on the H-terminated Si(001) surface [1]. Based on density-functional theory calculations, a new growth mechanism of the 1D acetylacetone line is proposed [2], which involves the radical chain reaction initiated at two dangling-bond sites on one side of two adjacent Si dimers. It is also enabled that, if an H-free Si dimer were employed as the initial reaction site, a 1D acetylacetone line can grow along the dimer row. Our findings represent the first insight into the growth of 1D molecular lines not only across but also along the dimer rows on the H-terminated Si(001) surface.

[1] Jin-Ho Choi and Jun-Hyung Cho, Physical Review Letters 102, 166102 (2009).

[2] Jin-Ho Choi and Jun-Hyung Cho, Physical Review Letters, submitted.

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