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One dimensional growth of styrene on H-Si(001)-(31): a Density Functional Theory study. NOBORU TAKEUCHI, CCMC-UNAM, ANNABELLA SELLONI, Dept. of Chemistry, Princeton University — Recent experimental work on the addition of styrene on hydrogenated Si (001) and (111) surfaces has provided evidence for a surface chain reaction mechanism initiated at isolated H vacancies. In contrast with the island-type growth on the H-terminated Si(111) surface, styrene is found to form one dimensional lines on the hydrogenated Si(001) surfaces. Using periodic Density Functional Theory (DFT) calculations, together with a recently developed method to find reaction pathways, we have studied the initial steps of the radical chain mechanism on the H-Si(001)-(3 $\times$1) surface. Our results suggest a preference for a one dimensional growth in the direction perpendicular to the Si dimer rows, in agreement with experiment. This preference is partly due to a smaller activation energy for hydrogen abstraction from the nearest dihydride site compared with hydrogen abstraction from a neighboring dimer, as well as to a strong repulsion between hydrogen atoms of the styrene molecules and monomer sites, when the growth is parallel to the dimer rows.

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