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Molecular Functionalization Mechanism of Hydrogenated Si Surfaces YOSUKE KANAI, Princeton University, ANNABELLA SELLONI, Princeton University, NOBORU TAKEUCHI, Universidad Nacional Autonoma de Mexico, ROBERTO CAR, Princeton University — Within the current effort to understand and develop the organic functionalization of silicon surfaces, recent experiments have identified the radical chain reaction of unsaturated organic molecules with H-terminated silicon surfaces as a particularly promising route for controlled formation of such functionalized surfaces. Using periodic Density Functional Theory calculations, we theoretically study and characterize the basic steps of the radical chain reaction mechanism for different (conjugated and unconjugated) aldehyde molecules reacting with the H-Si(111) surface, under the assumption that a Si dangling bond is initially present on the surface. Molecular conjugation is found to play a crucial role in the viability of the reaction, by controlling the delocalization of the spin density at the reaction intermediate. Interesting differences are observed and discussed between our present results for aldehydes and our previous study for the reactions of alkene/alkyne molecules with H-Si(111) [Takeuchi, et al *J. Am. Chem. Soc.* **2004**, *126*, 15890.]

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