Passivation and Secondary Functionalization of Allyl-Terminated Si(111) Surfaces

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Supporting Information

1. Computational model of surface 1
2. XPS comparing surfaces 1 and 2 after treatment by Route A
3. XPS illustrating the relative oxidation of surfaces 1 and 2 after treatment by Route A
Figure S.1. Energy-minimized molecular mechanics model of surface 1, indicating the variety of environments which the terminal olefins may inhabit, as well as the space enabling secondary reactions that is provided by the less-than 100% coverage. All atoms are scaled to their van der Waals radii. This calculation was performed in the Cerius² program (Accelrys) using the Universal force field and periodic boundary conditions with a $2 \times 2$ cell.
2. XPS comparing surfaces 1 and 2 after treatment by Route A

**Figure S.2.** XPS of surfaces 1 and 2, before and after treatment by the Heck reaction conditions. Note the increased amount of contamination of surface 2 after treatment, and the smaller F 1s peak, in comparison to surface 1 after treatment.
3. XPS illustrating the relative oxidation of surfaces 1 and 2 after treatment by Route A

![Graph showing XPS of Si 2p region of surfaces 1 and 2 before and after treatment by Route A]

**Figure S.3.** XPS of the Si 2p region of surfaces 1 and 2 before and after treatment by Route A, the Heck reaction. The SiO$_x$ peak, equivalent to 50% of a monolayer, is noticeable on both surfaces 1 and 2 after treatment in equal amounts. A shift in binding energy is observed between surfaces 1 and 2.