Supporting Information: Reaction of Dichlorophenylborane with H-Si(100)

Esther Frederick[a]‡ *, Quinn Campbell[a]‡, Angelica Benavidez[b], David R. Wheeler[a], Shashank Misra[a]*

AUTHOR ADDRESS

[a] Sandia National Laboratories, Albuquerque, NM, 87185

[b] University of New Mexico, Albuquerque, NM, 87131

Supporting Information

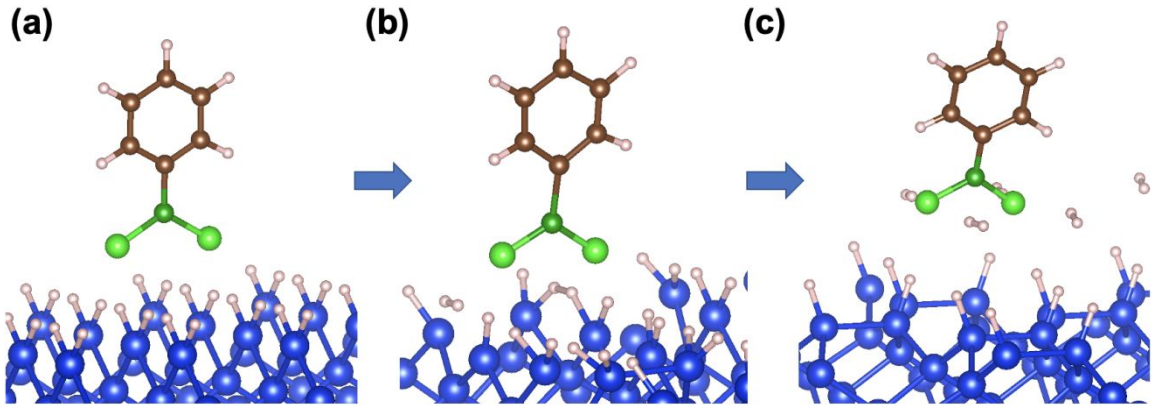

Figure S1. The pathway for physisorption of $PhBCl_2$ leading to a reconstruction of the Si(100) surface. (a) Initial positioning of $PhBCl_2$ on Si(100) surface, (b) a midpoint where long range interaction with the chlorine atoms has shifted terminating hydrogen molecules, (c) the final reconstructed Si(100)-2x1 surface.

For the DFT calculations in the main work, we largely assume a Si(100)-2x1 reconstruction of the surface. This is due to the tendency of the Si(100) surface to reconstruct within our calculations. In Figure S1 we show the typical pathway that leads to reconstruction. As the $PhBCl_2$ molecule approaches the Si(100) dihydride terminated surface, long range interaction between the chlorine and the hydrogen begin to shift the hydrogen termination structure of the surface. This eventually leads to a runaway effect, where half the hydrogen atoms desorb as H_2 molecules, and the surface reconstructs in a Si(100)-2x1, monohydride termination. While this is at least partially due to the small simulation size necessitated by DFT calculations, it is indicative of the general stability of the Si(100) surface. For simplicity, within the main work we therefore run all our calculations on a Si(100)-2x1, monohydride terminated surface. While this is not perfectly representative of reality, it provides a good qualitative understanding of $PhBCl_2$ interactions with a hydrogen terminated silicon surface.