

Supporting Information for

**Computational Study for Reactions of H Atoms with Adsorbed SiH₃
and Si₂H₅ on H-covered Si(100)-(2×1) Surface**

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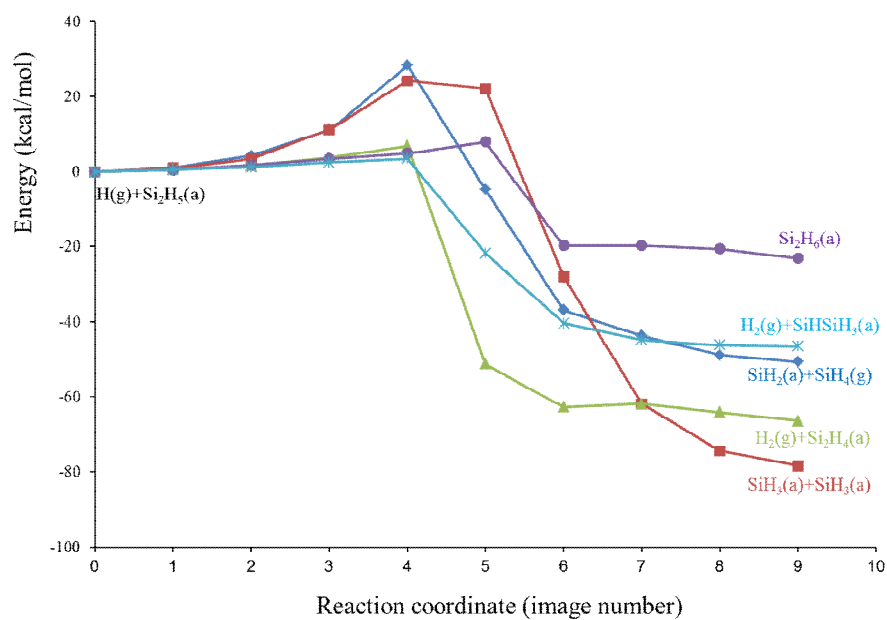


Figure S1. Minimum energy pathways for the reactions of $\text{H}(\text{g}) + \text{Si}_2\text{H}_5(\text{a})$ as the function of proper reaction coordinate.

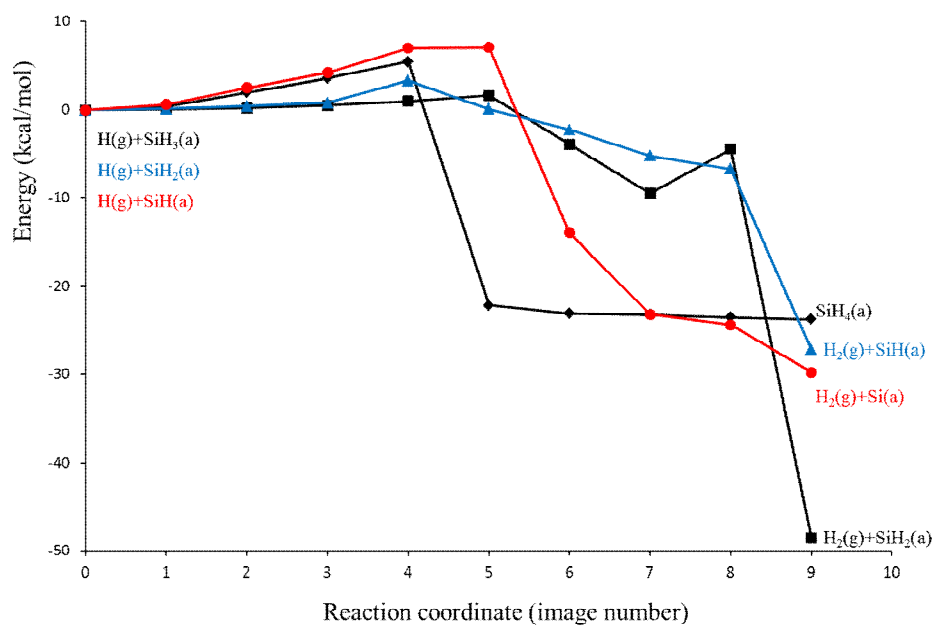


Figure S2. Minimum energy pathways for the reactions of $\text{H}(\text{g}) + \text{SiH}_x(\text{a})$, $x=1\sim3$, as the function of proper reaction coordinate.