## Supporting Information.

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| SAMPLE | $\mathrm{W}_{\text {adh }}\left(\mathrm{mJ} / \mathrm{m}^{2}\right)$ |
| :---: | :---: |
| $50 \%$ H-termination | 141 |
| $70 \%$ H-termination | 151 |
| $100 \%$ H-termination | 169 |

Figure SI.1. Still images are taken from an MD simulation of a flat $\operatorname{Si}(111)$ slab that was brought into contact with a flat H -terminated diamond (111) slab, with different amounts of H-termination.
(a) Illustration of the slab geometry. Rigid layer carbon and Si atoms and thermostated carbon and Si atoms are shown in blue and green, respectively. The remaining atoms are unconstrained, where carbon, hydrogen, and silicon are cyan, red, and yellow, respectively. (b) Force-distance curves for the Indent-Retract tests of the slabs with diamond hydrogen terminations of $50 \%, 70 \%$, and $100 \%$. Integrating force-distance curves with respect to distance provides the work performed. (c) A table of the resulting work of adhesion values.

