

Electronic Supplementary Information

Surface structural phase transition induced by formation of metal-organic network on Si(111)- $\sqrt{7} \times \sqrt{3}$ -In surface

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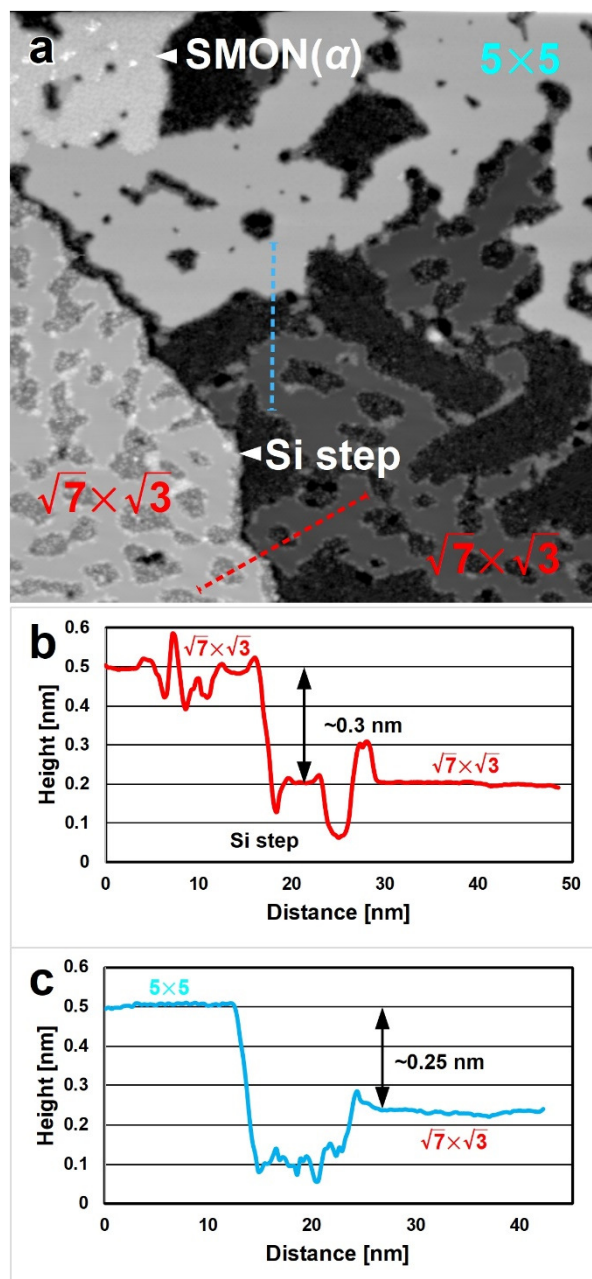


Figure S1 (a) STM image acquired after TCNQ deposition on the Si(111)- $\sqrt{7} \times \sqrt{3}$ -In surface. (b) and (c) show line profiles measured along the red and the blue dashed lines shown in (a), respectively. The height of a single atomic step on Si(111) is about 0.3 nm (as shown in (b)), while the measured height difference between a $\sqrt{7} \times \sqrt{3}$ and a 5×5 terrace is about 0.25 nm (as shown in (c)). Image size of (a) is $148 \times 148 \text{ nm}^2$.

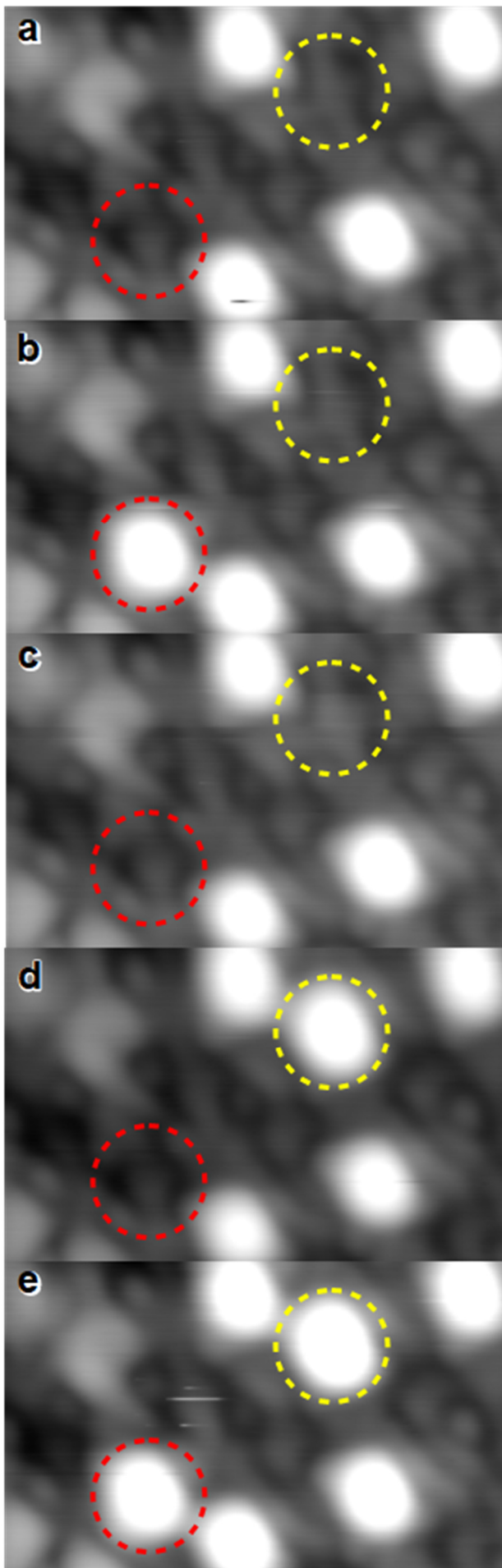


Figure S2 Five STM images extracted from successive scans taken at the same sample position. Bright humps are disappearing and reappearing at the positions marked by red and yellow circles.

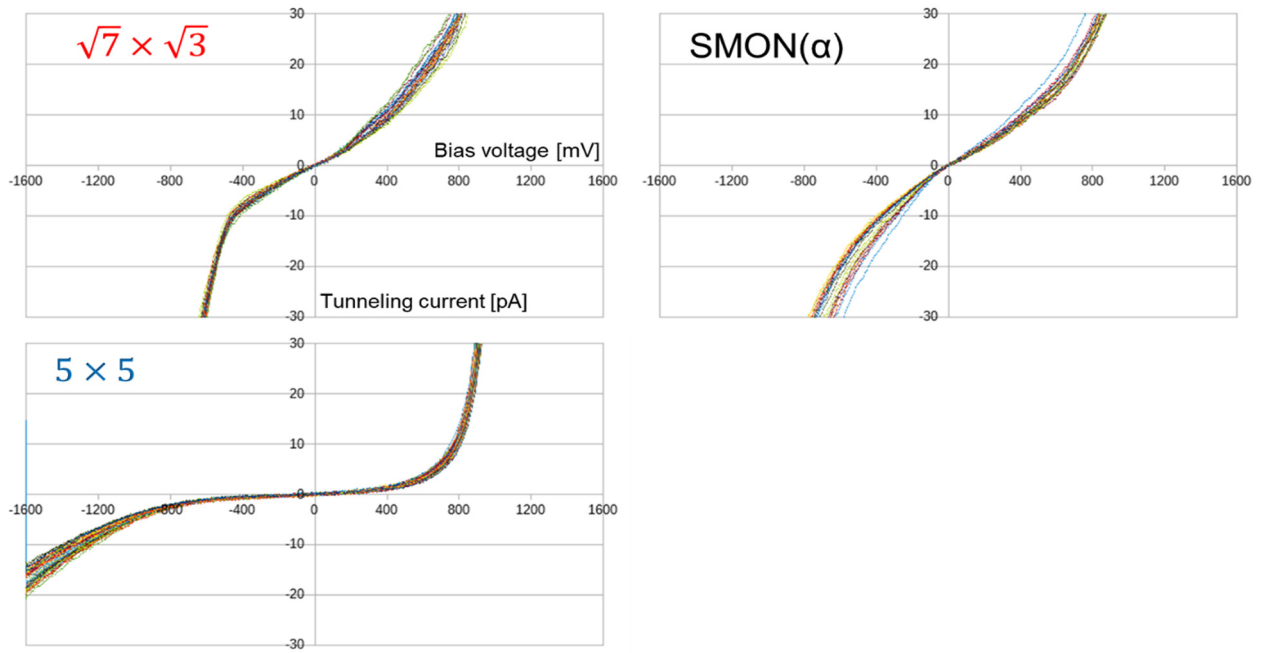


Figure S3 I-V curves measured on the $\sqrt{7} \times \sqrt{3}$ reconstruction, on the SMON(α), and on the 5×5 reconstruction. The 5×5 reconstruction is more insulating than the others close to the Fermi energy ($V = 0$).

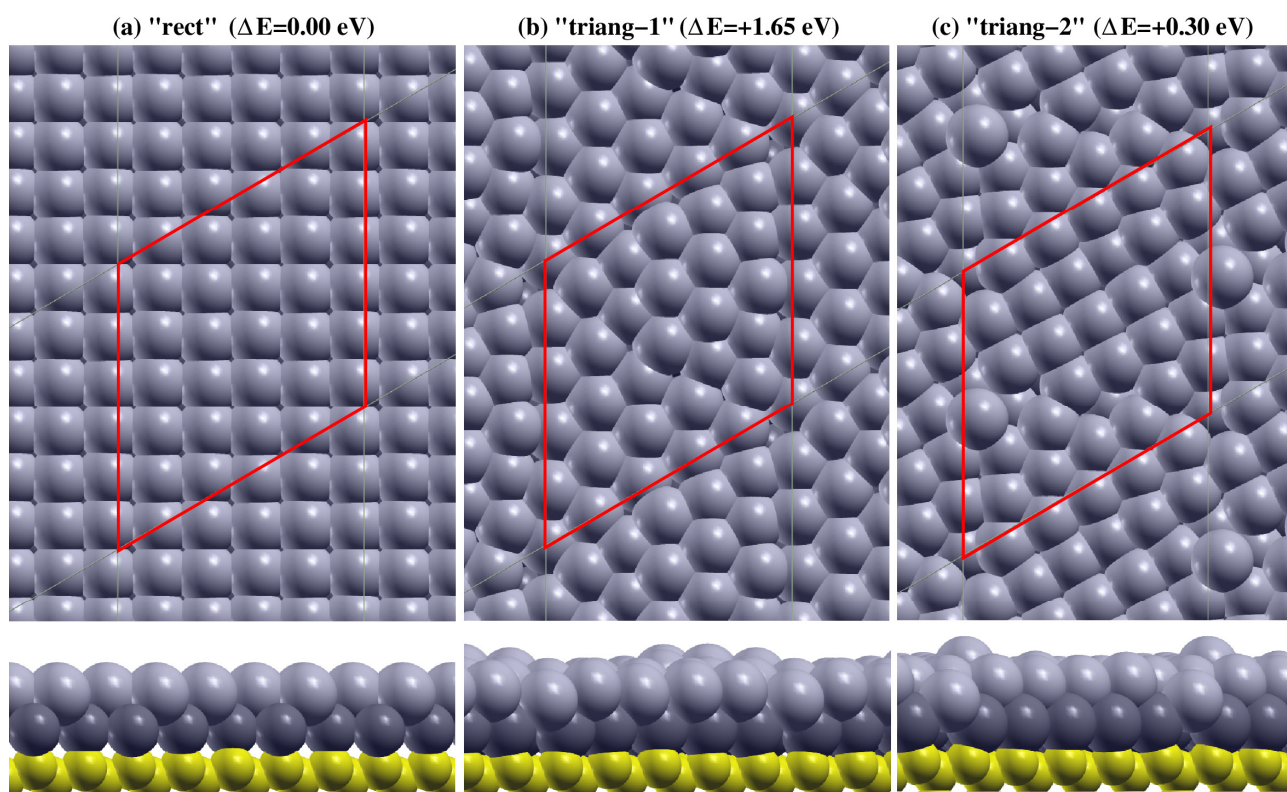


Figure S4 Top and side views (in SpaceFill display mode) of the (a) “rect”, (b) “triang-1” and (c) “triang-2” configurations with 2.4 ML In-coverage. Yellow spheres represent the Si atoms; bright/dark gray spheres represent top-/bottom-layer In atoms; red lines indicate the 5×5 surface unit cell. Relative total energies (ΔE) with respect to the “rect” configuration are shown at the top of each figure.

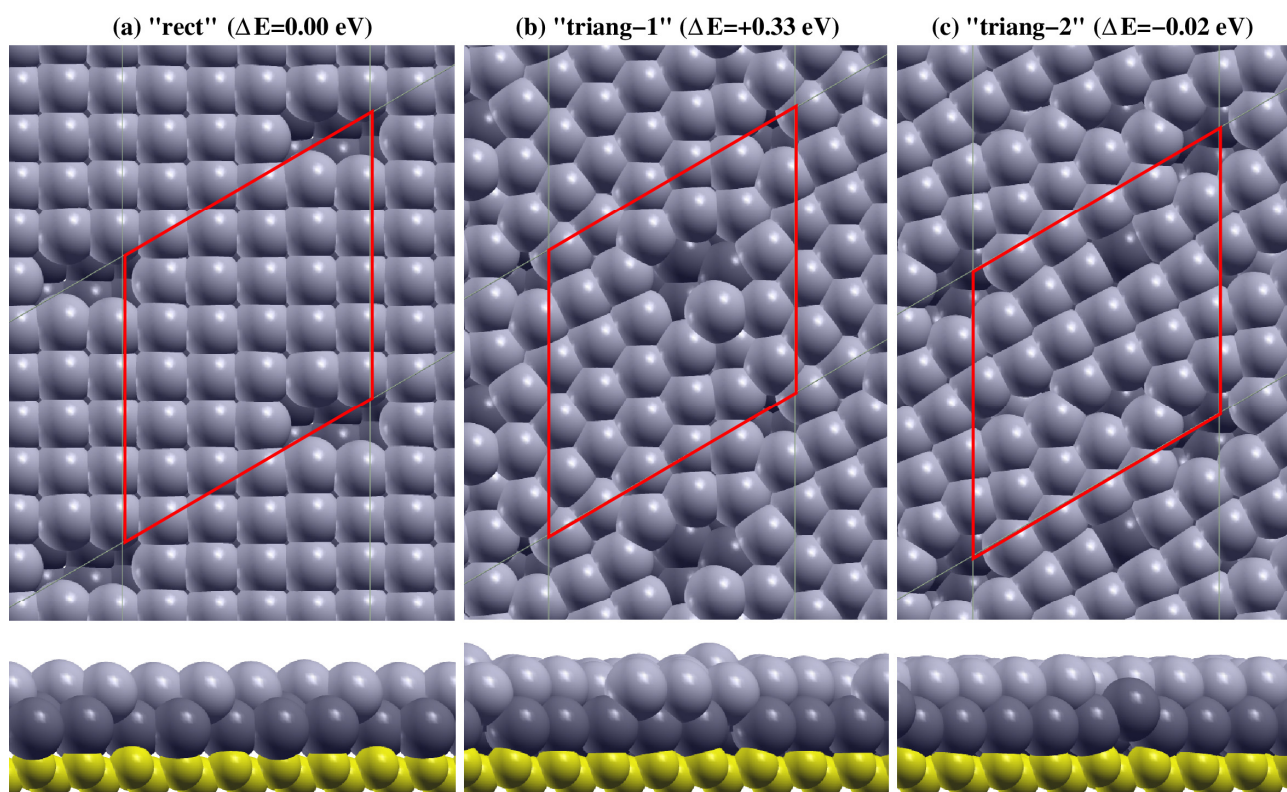


Figure S5 Top and side views (in SpaceFill display mode) of the (a) “rect”, (b) “triang-1” and (c) “triang-2” configurations with 2.32 ML In-coverage. Yellow spheres represent the Si atoms; bright/dark gray spheres represent top-/bottom-layer In atoms; red lines indicate the 5×5 surface unit cell. Relative total energies (ΔE) with respect to the “rect” configuration are shown at the top of each figure.

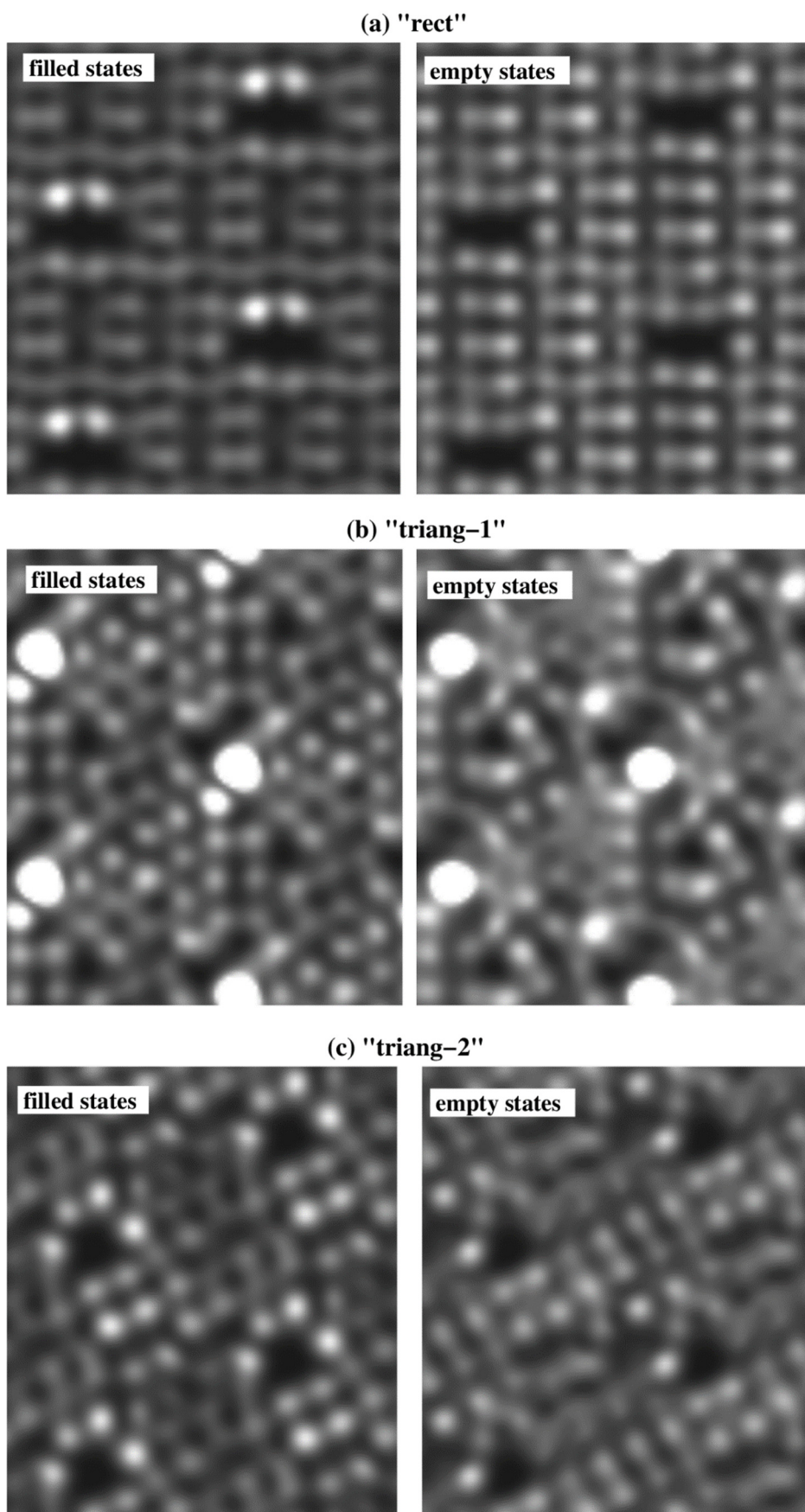


Figure S6 Simulated STM images (obtained at a constant density of $5 \times 10^{-3} \text{ \AA}^{-3}$) of the (a) "rect", (b) "triang-1" and (c) "triang-2" configurations with 2.32 ML In-coverage.

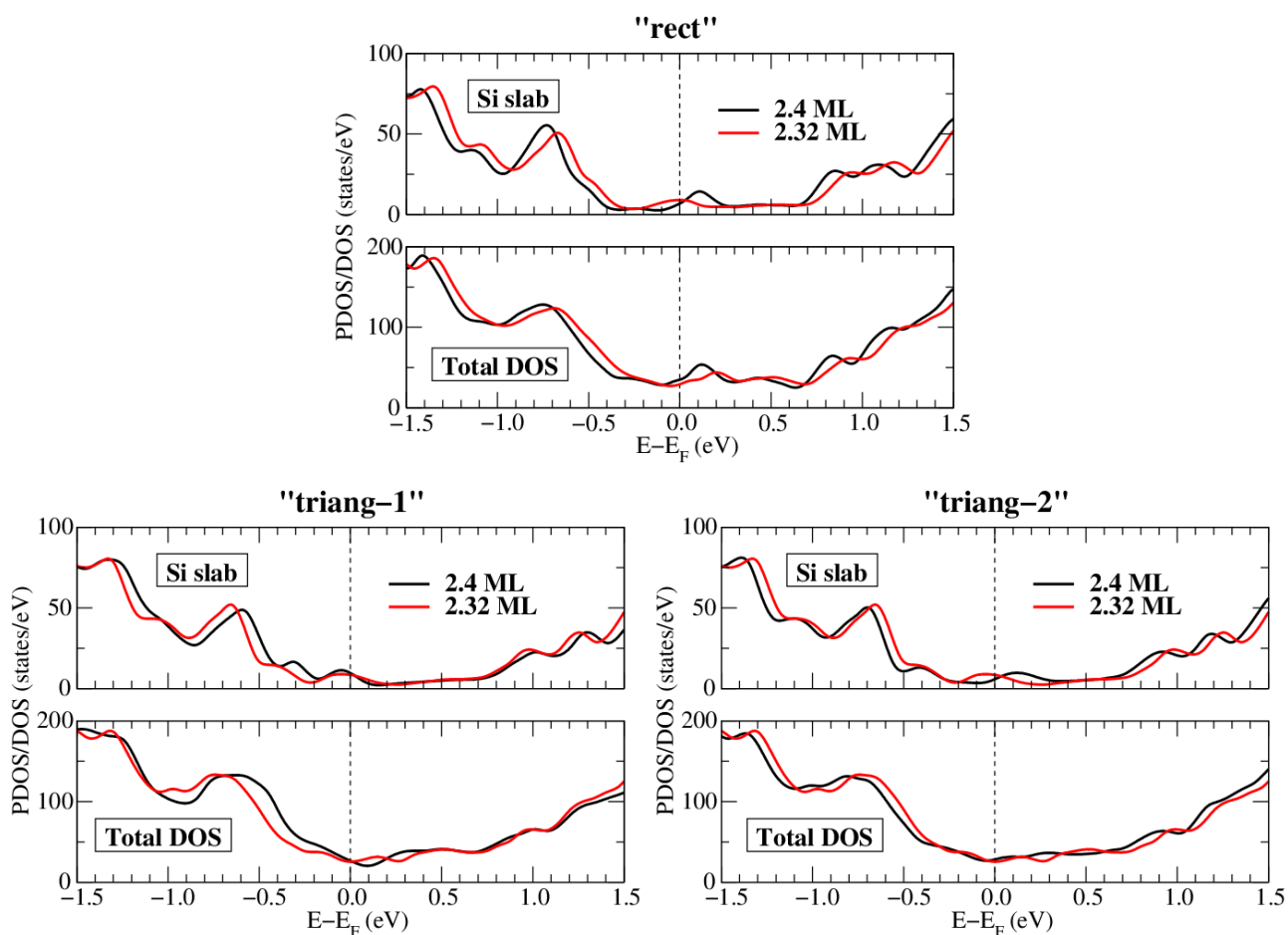


Figure S7 Projected (PDOS) and total density of states (DOS) for the “rect” and the two “triang” configurations with In-coverage of 2.4 and 2.32 ML. Top and bottom panels show PDOS of Si slab and total DOS, respectively.