

Supporting information for:

The Interactive Effect of Hysteresis and Surface Chemistry on Gated Silicon Nanowire Gas Sensors

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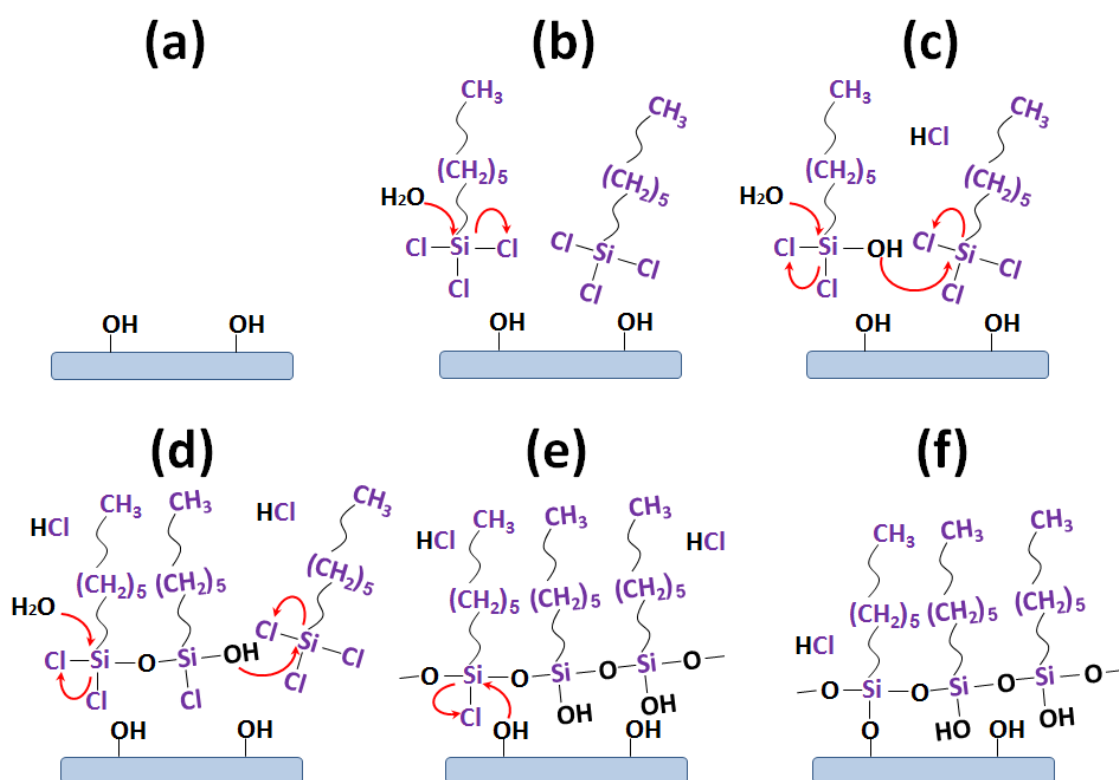


Figure 1S. A simplified scheme for the attachment of HTS monolayer – as a representative example for TS monolayers - to SiO₂/Si surface by the common and *direct self-assembly* procedure: SiO₂/Si surface with free hydroxyl (Si-OH) groups (a) is exposed to HTS in a chloroform (b). Water residues in the chloroform solution and/or on the SiO₂/Si surface replace the HTS's chlorine atoms by OH groups (c). Hydroxyl groups from adjacent HTS molecules react with each the other (d), and, also, hydroxyl groups from HTS molecules react with the Si-OH groups on the surface (e). The result of these reactions is cross-linked Si-O-Si bonds (e) and a monolayer that (partially) eliminates the Si-OH groups on the SiO₂/Si surface (f).

Extended Model Supported Analysis for Hysteresis versus Back-Gate Voltage:

The relative conductivity change of the OH^{low}-Si NW FET and OH^{high}-Si NW FET forward scans compared to the backward scan, $G_F - G_B / G_B$, could be formulated as follows:

$$G = q\mu_h \left(Q_S^v (V_{gs} - V_{th}) + \frac{2Q_{css}}{r_{nw}} - \frac{2Q_{trap}}{r_{nw}} \right) \quad (1S)$$

$$\frac{G_F^y - G_B^y}{G_B^y} \approx \frac{1}{\frac{r_{nw}}{2} \frac{Q_S^v (V_{bgs} - V_{th}^B)}{Q_{css}} + 1} \cdot \left(\frac{\mu_h^F Q_S^v (V_{th}^F) - \mu_h^B Q_S^v (V_{th}^B)}{2\mu_h^B Q_{css} / r_{nw}} - \frac{\mu_h^F Q_{trap}}{\mu_h^B Q_{css}} \right) \quad (2S)$$

where subscript 'y' stands for either 'OH^{low}' or 'OH^{high}'. For small Q_{trap} , equation (2S) reduces to Equation (20) because $V_{th}^F \approx V_{th}^B$ and $\mu_h^F \approx \mu_h^B$; therefore, the first part in equation (2S) brackets is negligible at high positive and negative back-gate voltages. The relative conductivity change of the HTS^c-Si NW FET and OH^{high}-Si NW FET backward scans compared to the OH^{low}-Si NW FET backward scan, $G_x - G_{OH^{low}} / G_{OH^{low}}$, could be formulated as follows:

$$G = q\mu_h \left(Q_S^v (V_{gs} - V_{th}) + \frac{2Q_{css}}{r_{nw}} \right) \quad (3S)$$

$$\frac{G_x - G_{OH^{low}}}{G_{OH^{low}}} \approx \frac{-1}{\frac{r_{nw}}{2} \frac{Q_S^v (V_{bgs} - V_{th}^{OH^{low}})}{Q_{css}^{OH^{low}}} + 1} \cdot \left(\frac{\mu_h^x Q_S^v (V_{th}^x) - \mu_h^{OH^{low}} Q_S^v (V_{th}^{OH^{low}})}{2\mu_h^{OH^{low}} Q_{css}^{OH^{low}} / r_{nw}} + \frac{\mu_h^x Q_{css} - \mu_h^{OH^{low}} Q_{css}^{OH^{low}}}{\mu_h^{OH^{low}} Q_{css}^{OH^{low}}} \right) \quad (4S)$$

where subscript 'x' stand for 'HTS^c' or 'OH^{high}'

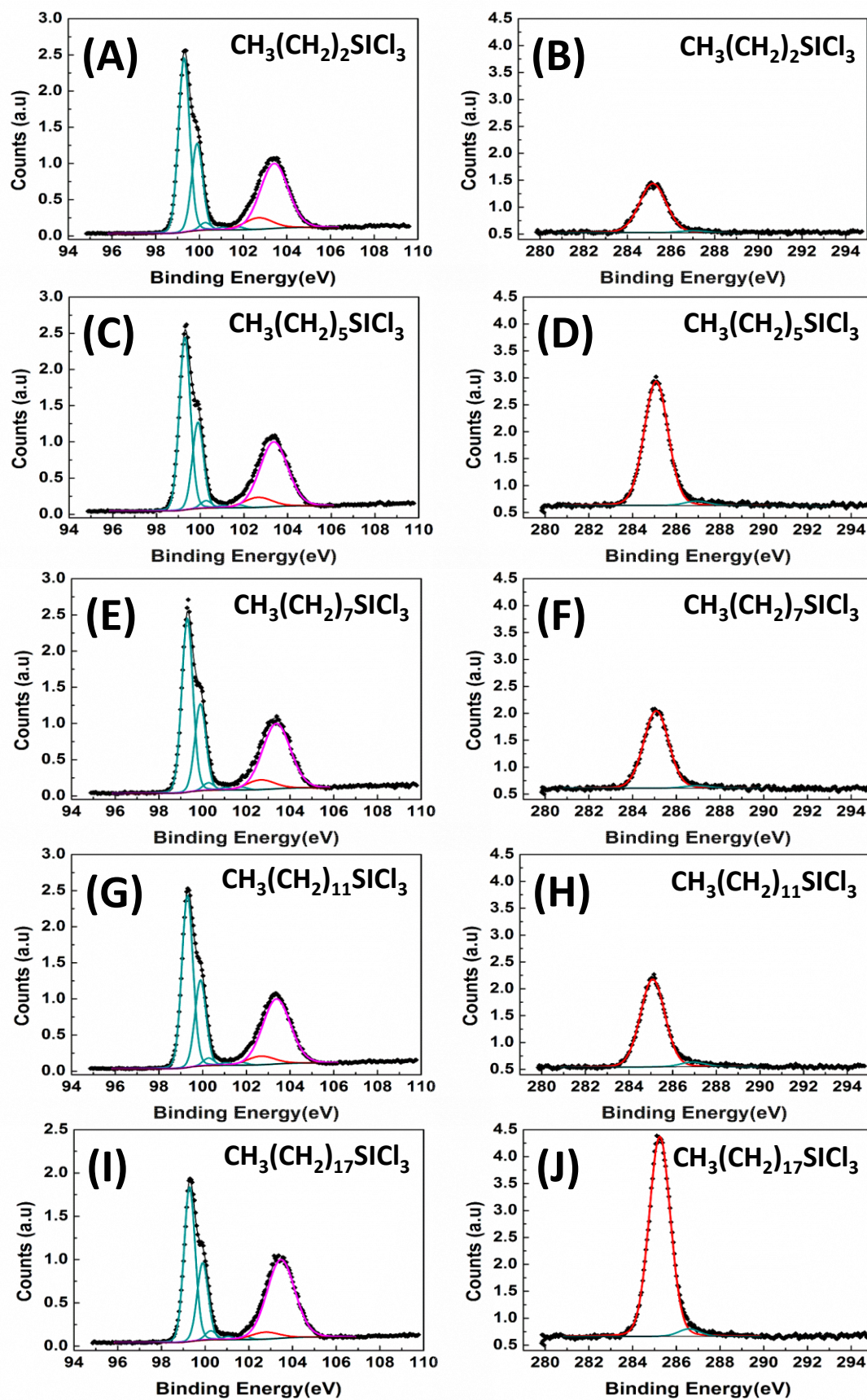


Figure 2S. Normalized XPS Si_{2p} (left column, A,C,E,G,I) and C_{1s} (right column B,D,F,H,J) spectra of five TS^c molecules - $\text{CH}_3(\text{CH}_2)_n\text{SiCl}_3$ - differing in their carbon chain length: (A&B) $n+l=3$; (C&D) $n+l=6$; (E&F) $n+l=8$; (G&H) $n+l=12$; (I&J) and $n+l=18$.

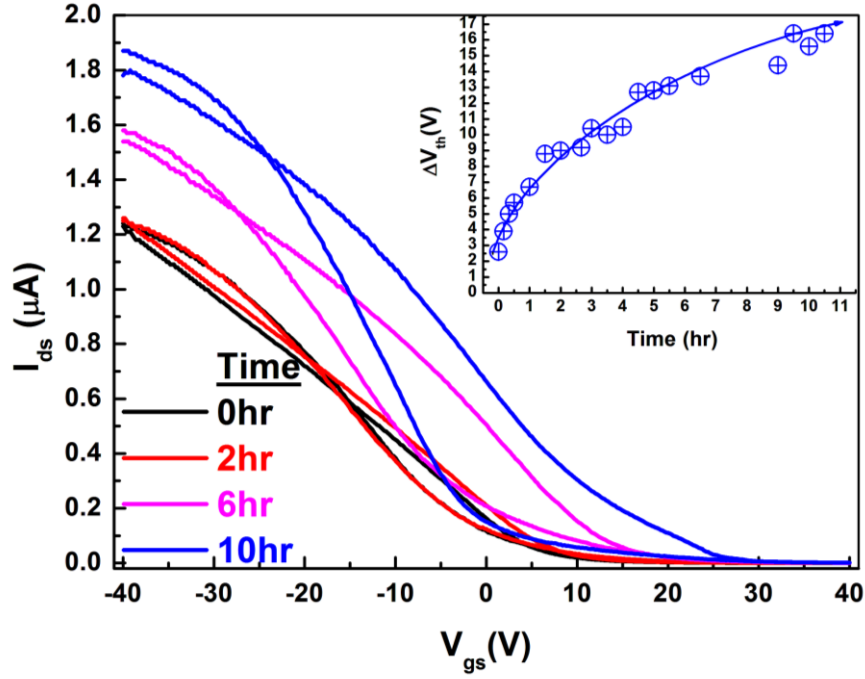


Figure 3S. Typical I_{ds} - V_{gs} characteristics of OH^{low} -Si NW FET on extended exposure periods to 15% RH. **Inset:** ΔV_{th} as a function of time for the same device; the measurement was stopped instantly if a film of condensed water was seen.

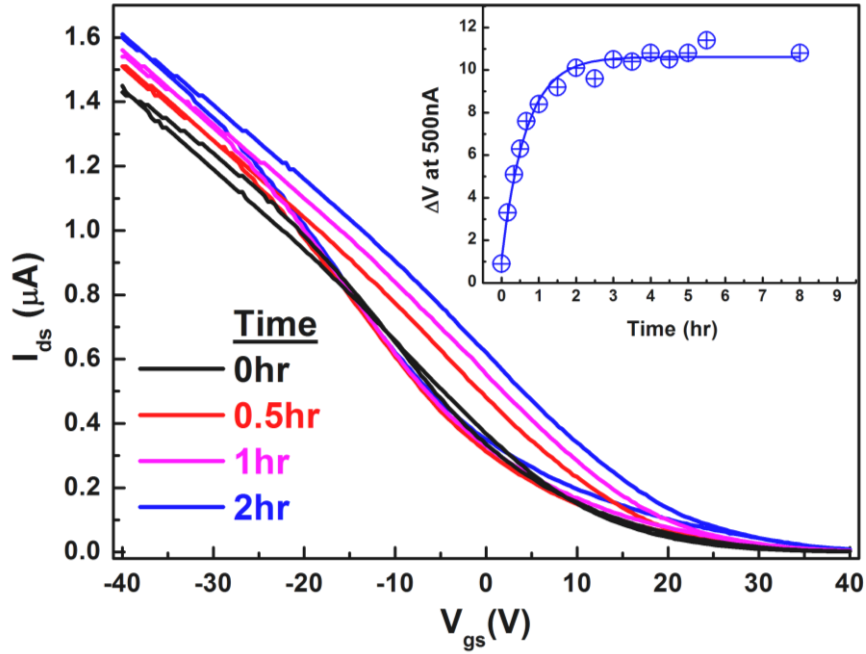


Figure 4S. Typical I_{ds} - V_{gs} characteristics of HTS^{uc} -Si NW FET on extended exposure periods to 15% RH. **Inset:** ΔV_{th} as a function of time for the same device; the measurement was stopped instantly if a film of condensed water was seen.

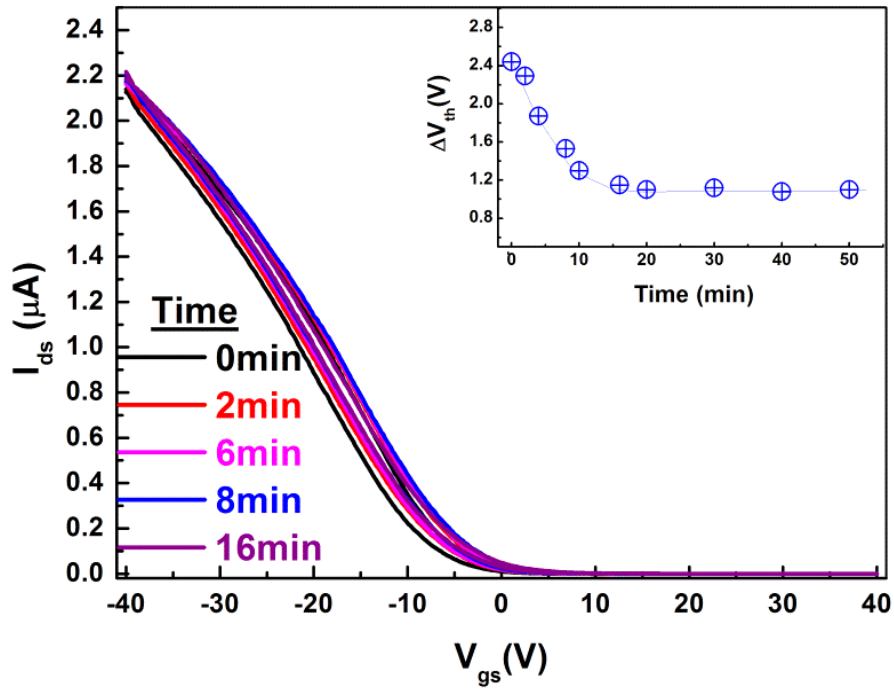


Figure 5S. Typical I_{ds} - V_{gs} characteristics of HTS^c-Si NW FET on extended exposure periods to 15% RH. **Inset:** ΔV_{th} as a function of time for the same device.