Click Chemistry in Ultra-high Vacuum – Tetrazine Coupling with Methyl Enol Ether Covalently Linked to Si(001)

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I. N 1s spectra of tetrazine adsorbed on MEECO-covered Si(001)

Figure S1: (a) N 1s spectra from a tetrazine multilayer adsorbed on a MEECO covered Si(001) surface at 150 K (same experiment as shown in Fig. 2(a) in the main paper). (b) After heating to 300 K (30 min), no N 1s signal is observed any more, all tetrazine molecules are desorbed. No reaction neither with the MEECO nor with the surface has taken place. The latter indicates sufficient passivation by the adsorption of MEECO with respect to direct adsorption of tetrazine on Si(001).

II. Computational raw data

Computational raw data is available at the NOMAD repository:
https://dx.doi.org/10.17172/NOMAD/2020.11.19-1