

Supporting Information

Proton-detected Multidimensional Solid-State NMR Enables Precise Characterization of Vanadium Surface Species at Natural Abundance

Deni Mance, Aleix Comas-Vives, Christophe Copéret**

Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog Weg 1-5, CH-8093 Zürich, Switzerland

*Email: mance@inorg.chem.ethz.ch.

*Email: ccoperet@ethz.ch

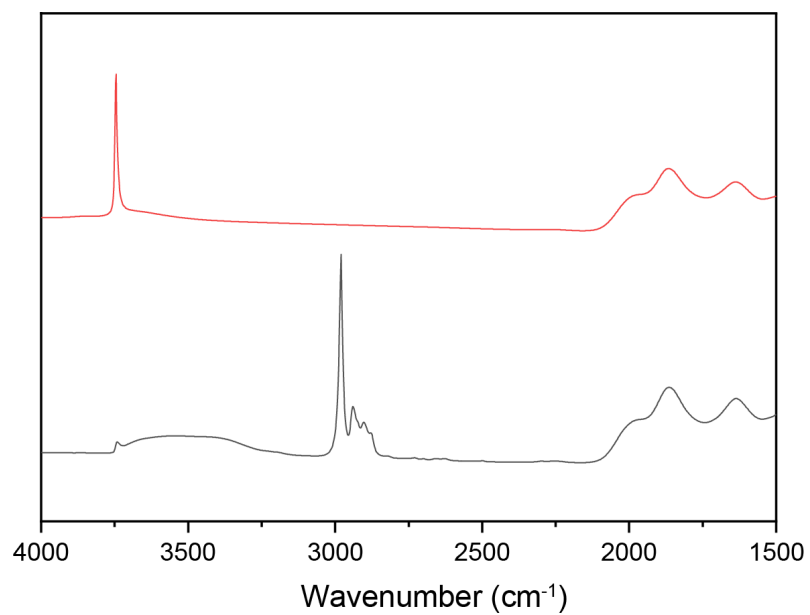


Figure S1. FTIR recorded in transmission mode with in red the spectrum of dehydroxylated silica at 700°C and in black the spectrum after grafting vanadium oxytriisopropoxide onto the dehydroxylated silica

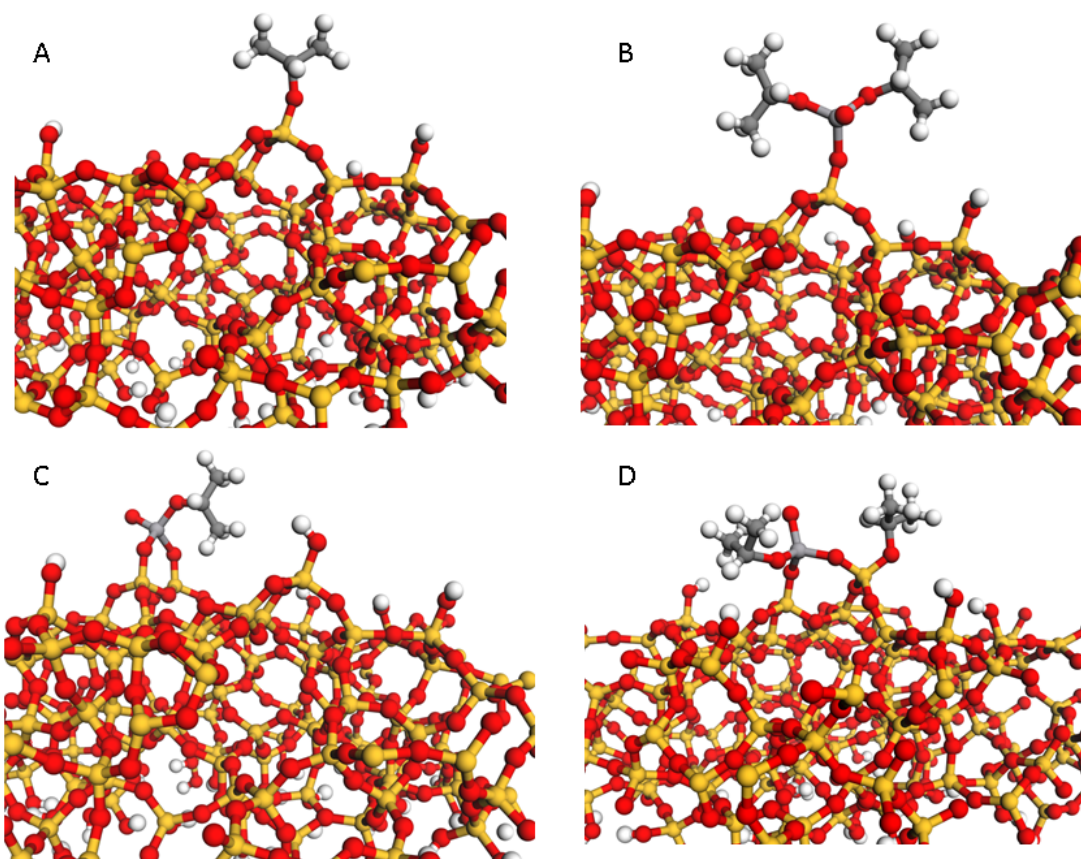


Figure S2. Geometry optimized surface structures using VASP. A) OiPr, B) single sites $\text{VO}(\text{OiPr})_2$, C) bis-grafted $\text{VO}(\text{OiPr})$ and D) bis-grafted $\text{VO}(\text{OiPr})$ within presence of OiPr modeled on dehydroxylated silica.