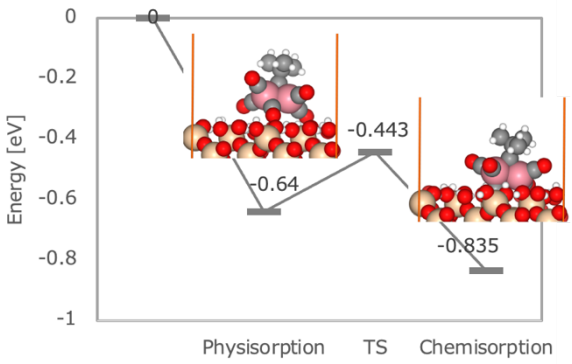

Fig. 1. Proposed adsorption pathway of a gas-phase–activated CCTBA fragment on OH-terminated SiO_2.
The potential energy profile highlights a metastable physisorbed precursor complex and the subsequent structural rearrangement leading to Co–O bond formation. Representative snapshots (initial approach → physisorbed state → transition state → chemisorbed product) visualize how the fragment is oriented and captured at the surface, clarifying the reaction coordinate responsible for nucleation on the nominal non-growth surface (energetic annotations are given on the profile).

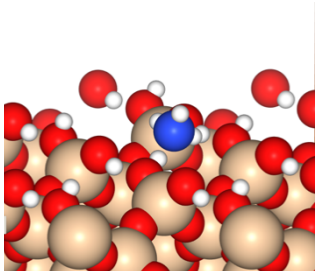

Fig. 2. NH_3 adsorption geometry on OH-terminated SiO_2 and site-blocking concept.
Optimized structures illustrate that NH_3 is stabilized at specific surface hydroxyl motifs via directional hydrogen bonding, forming a localized "cap" over the reactive OH site. The annotated contact distances and orientation clarify how this adsorption configuration can sterically and electronically hinder access of the Co-precursor fragment to the same site.