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The interaction of carbon monoxide with clean and surface-modified zinc oxide nanoparticles: A UHV-FTIRS study

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ABSTRACT

The interaction of CO with differently modified polycrystalline ZnO has been studied by FTIR spectroscopy under ultrahigh vacuum conditions (UHV-FTIRS). After exposing the clean, adsorbate-free ZnO nanoparticles to CO at 110 K we observe an intense vibrational band at 2187 cm^{-1} which is assigned to a majority of CO species bound to the Zn^{2+} sites on the mixed-terminated $\text{ZnO}(10\bar{1}0)$ surface. After the exposure of CO_2 -pretreated ZnO nanoparticles to CO at 110 K, a new CO band is observed at 2215 cm^{-1} , which originates from CO species adsorbed on the “free” Zn sites embedded within the (2×1) tridentate carbonate structure on the $\text{ZnO}(10\bar{1}0)$ surface. UHV-FTIRS data recorded at different sample temperatures demonstrate that the binding energy of CO on polycrystalline ZnO is substantially increased in the presence of pre-adsorbed CO_2 . The presence of hydroxyl species on the ZnO powder particles does not lead to substantial changes of the CO vibrational bands detected at 110 K under UHV conditions.

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