The identification of hydroxyl groups on ZnO nanoparticles by infrared spectroscopy

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The interaction of water with ZnO nanoparticles has been studied by means of diffuse reflectance infrared spectroscopy (DRIFTS) and ultra-high vacuum FTIR spectroscopy (UHV-FTIRS). Exposing clean ZnO powder to water at 323 K leads to both molecular and dissociative adsorption of H_2O forming a number of hydroxyl species. All the OH bands are clearly identified by the adsorption of D_2O showing the expected isotopic shifts. According to the vibrational and thermal stability data obtained from single crystal surfaces, the OH species observed on ZnO nanoparticles are identified as follows: (1) OH group (3620 cm^{-1}) on the polar O–ZnO(000$\bar{1}$) surface formed *via* dissociation of water on oxygen vacancy sites; (2) partial dissociation of water on the mixed-terminated ZnO(10$\bar{1}$0) surface yielding coexistent H_2O ($\sim$3150 and 3687 cm^{-1}) and OH species (3672 cm^{-1}), where the molecularly adsorbed H_2O is further identified by the characteristic scissoring mode at 1617 cm^{-1}; (3) isolated OH species (3639 and 3656 cm^{-1}) formed on the mixed-terminated ZnO(10$\bar{1}$0) surface; (4) interaction of water with defects forming hydroxyl (or O–H$\cdots$O) species (3564 and 3448 cm^{-1}).