

He-atom scattering (HAS), X-ray photoelectron spectroscopy (XPS and NEXAFS), periodic density functional theory and quantum chemical ab initio cluster calculations have been used for characterizing the adsorption of CO<sub>2</sub> on the mixed terminated ZnO(10-10) surface. The HAS data allow to identify three different structural phases of CO<sub>2</sub> in the monolayer regime: A high-density (1×1) phase at low temperature, a lower density (2×1) phase at higher temperatures, and in addition an incommensurate phase (which has not been reported before) with a slightly lower coverage and a 2.3-fold periodicity at surface temperatures above 270 K. XPS and NEXAFS measurements performed for the two low-coverage phases show that CO<sub>2</sub> is adsorbed in form of a carbonate species. This is supported by the ab initio calculations for CO<sub>2</sub> adsorbed on ZnO(10-10). The calculated XP and NEXAFS spectra agree with the experimental data and are only compatible with an adsorbed carbonate species, the presence of physisorbed CO<sub>2</sub> can be excluded. In addition, the calculations demonstrate that X-ray emission spectroscopy (XES) is a sensitive method to distinguish between linear CO<sub>2</sub> and carbonate.