Structure and dynamics of CO overlayers on a hydroxylated metal oxide: The polar ZnO(000$\bar{1}$) surface

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Abstract

The adsorption and desorption of CO on the hydroxylated, O–terminated polar ZnO(000$\bar{1}$) surface has been studied using He–atom scattering. The experimental results reveal the formation of a physisorbed ordered CO overlayer. In addition to recording angular distributions of elastically scattered He atoms, also the dynamical properties of the CO overlayer have been investigated using inelastic He–atom scattering. With the aid of electronic structure calculations a loss peak with an energy transfer of 7.2 meV is assigned to the frustrated translation of the CO molecule normal to the surface.