Ab initio studies of the adsorption of CO on the $Cr_2O_3(0001)$ surface

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The adsorption of CO on the polar $Cr_2O_3(0001)$ surface was studied by quantum-chemical ab initio cluster calculations. A full four-dimensional potential for the interaction of a single CO molecule with the surface was calculated and fitted to an analytic function containing electrostatic and Lennard-Jones type terms. The geometric structure of the adsorbed monolayer is also considered and good agreement with the experimental ARUPS data is found. Shifts of the orbital energies and vibrational stretch frequency of the adsorbed CO were calculated and used for the interpretation of the mesured UP and IRAS spectra.