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## Abstract

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## Adsorbate structure modeling based on electron energy loss spectroscopy and lattice dynamical calculations: Application to O/A1(111).



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Available online 5 November 2001.

## Abstract

High-resolution electron energy loss spectroscopy (EELS) and lattice dynamical calculations based on pair interactions are used to investigate oxygen chemisorption on Al(111). The O/Al(111) System is complicated by the simultaneous formation of an oxygen overlayer and underlayer. Oxygen atoms at overlayer and underlayer sites near the Al(111) surface produce well-defined vibrational loss peaks in EELS spectra, however, dynamical coupling between the oxygen atoms and with the host lattice cause vibrational energies to shift with overlayer and underlayer concentrations. These shifts as well as structural parameters of the O/Al(111) complex can be deduced from a slab model of the surface lattice dynamics.

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