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Theory of Auger decay for fine surface structure features. GIAN
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SEBASTIANO CARAVATI, Universita' di Milano-Bicocca — We calculate the core-
core-valence (CCV) Auger profiles of an adatom on a periodic surface within the
DFT framework by using a method based on the local density of states (LDOS),
with a core hole on the atom, in the neighbourhood of the impurity. We investigate
the CCV lineshapes of Na on Al(111) for the two ordered phases observed at room
temperature. From a detailed comparison of the calculated spectra with specific
recent experiments for the KL_{23} lineshape of Na, we prove that a theoretical effort
(based on DFT) can allow for determining the fine details of the two surface geome-
tries of the adsorbate system, and also for unravelling components from inequivalent
adatoms coexisting in the signal.

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