

**Multilayer Relaxation of Al(100) and Al(110) Surface: An ab initio Pseudopotential Study**

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The multilayer relaxations of Al(100) and Al(110) surface are studied using the plane wave ab initio pseudopotential method within the local density functional theory. Our calculations show that the surface relaxation of Al(100) is an "anomalous" outward relaxation (1.89%), and is in excellent agreement with published experimental results (1.8%). This is in contrast to several previous empirical and semi-empirical theoretical studies whose predictions are in contradiction with experiments. For the Al(110) surface, our results show inward relaxation, which is consistent with experiments (LEED) and other theoretical calculations. The origin of "inward" and "outward" relaxation is discussed. The surface energy and surface electronic properties are also studied in this work.