

A Model for Surface States and Catalysis on *d*-Band Perovskites*

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A qualitative model will be discussed which suggests that the catalytic activity of *d*-band perovskites such as (reduced) SrTiO_3 , RCoO_3 (R = rare earth atom) and mixed compounds such as $\text{La}_{1-x}\text{Pb}_x\text{MnO}_3$ can be interpreted in terms of localized orbital symmetry concepts.

The major barriers which inhibit certain

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classes of chemical reactions and the role of the *d*-electron in removing these barriers will be discussed. The essential features of the energy bands of *d*-band perovskites will be reviewed in terms of a simple LCAO model which gives quantitative results for both bulk and surface electronic states. Using this model we present a qualitative discussion of catalytic activity including the roles of surface density of states, surface defects, and surface electrostatic potentials.