Thermodynamic Stability of the $CaMnO_3$ (001) Surface

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Relative thermodynamic stability of surface reconstructions, consisting of vacancies, adatoms and additional layers, in both CaO and MnO_2 terminations is calculated to predict the surface phase diagram of $(\sqrt{2} \times \sqrt{2})R45^\circ$ $CaMnO_3$ (001) using *ab initio* thermodynamics. It is found that MnO_2-based surfaces are dominant within the stability region as temperature is introduced to the secondary phases boundary conditions. The magnetic ordering effects on the surface stability of $CaMnO_3$ are explored leading to significant changes in MnO_2 terminated surface phase diagram.

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