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Methanol Adsorption and Dissociation on LaMnO<sub>3</sub> and Sr Doped LaMnO<sub>3</sub> (001) Surfaces

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## Highlights

- DFT study of methanol adsorption and dissociation on  $\text{MnO}_2$  and LaO terminated  $\text{LaMnO}_3$  (001) surfaces as a function of Sr dopant enrichment
- Electron depletion in negatively charged  $\text{MnO}_2$  surface layer enhanced by Sr doping
- Electron accumulation in positively charged LaO surface layer reduced by Sr doping
- Dissociative methanol adsorption strongly preferred on LaO termination over  $\text{MnO}_2$  termination in  $\text{LaMnO}_3$  and moderately doped  $\text{LaMnO}_3$
- For highly Sr enriched surfaces, methanol favors dissociative adsorption on  $\text{MnO}_2$  termination over LaO termination

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