Methanol Adsorption and Dissociation on $LaMnO_3$ and Sr Doped $LaMnO_3$ (001) Surfaces

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Highlights

- DFT study of methanol adsorption and dissociation on MnO_2 and LaO terminated $LaMnO_3$ (001) surfaces as a function of Sr dopant enrichment
- Electron depletion in negatively charged 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 MnO_2 termination in $LaMnO_3$ and moderately doped $LaMnO_3$
- For highly Sr enriched surfaces, methanol favors dissociative adsorption on MnO_2 termination over LaO termination