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First Principles Investigation of Reversible Adsorption/Desorption and Molecular Dissociation of CO_2 on Ferroelectric $PbTiO_3$-supported ZnO Thin Films BABATUNDE ALAWODE, ALEXIE KOLPAK, Massachusetts Institute of Technology, Cambridge MA 02139, KOLPAK GROUP TEAM — Applying an electric field across a ferroelectric changes its polarization direction. When epitaxial layers are grown on such materials, the polarization may induce new atomic configurations at the interface. In this paper, we use density functional theory calculations to demonstrate that this effect can be used to reversibly modify the surface chemistry of thin ZnO grown on ferroelectric $PbTiO_3$. We show that both the substrate polarization direction and the thickness of the ZnO film have a significant effect on the adsorption energy of CO_2 and methanol, indicating that dynamic polarization switching could be used to minimize reaction barriers and/or enhance selectivity. As an example, we demonstrate a pathway for thermal CO_2 dissociation over a single monolayer of ZnO on $PbTiO_3$ with a predicted reaction rate several orders of magnitude higher than that over unsupported ZnO. Our results suggest that ferroelectric-supported ZnO, and dynamically tunable catalysts in general, could enable lower-energy approaches for CO_2 conversion.

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