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$ZnO/PbTiO_3$ as a Novel Catalyst for CO_2 Conversion BABATUNDE ALAWODE, ALEXIE KOLPAK, Massachusetts Institute of Technology, Cambridge, MA — Due to its role in climate change, there is a great interest in finding ways to take advantage of the vast amount of waste CO_2 we produce by its conversion to useful substances. This is currently impractical due to the high temperatures and pressures generally required for the synthesis of compounds using CO_2 as a precursor. To make direct CO_2 capture and conversion economically viable, new materials able to catalyze the conversion reactions at significantly milder conditions will be essential. In this work, we use DFT computations to design a dynamically tunable ferroelectric oxide-supported thin film catalyst that can capture CO_2 directly from the emission stream and convert it into methanol or cyclic carbonates. One promising candidate for a dynamically tunable catalyst of this type is $Zn_xO_y/PbTiO_3$. We demonstrate that switching the polarization of the ferroelectric substrate substantially changes the surface atomic and electronic properties of the heterostructure, thereby enabling tunable absorption. We investigate reaction pathways on unsupported and supported ZnO for common CO_2 reactions. Our approach may lead not only to new technologies for reducing emissions, but also to novel catalysts that could decrease energy consumption for industrial-scale synthetic processes.

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